



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:13 AM UTC

PDB ID : 4R1R / pdb_00004r1r
Title : RIBONUCLEOTIDE REDUCTASE R1 PROTEIN WITH SUBSTRATE,
GDP AND EFFECTOR DTTP FROM ESCHERICHIA COLI
Authors : Eriksson, M.; Eklund, H.
Deposited on : 1997-07-22
Resolution : 3.20 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

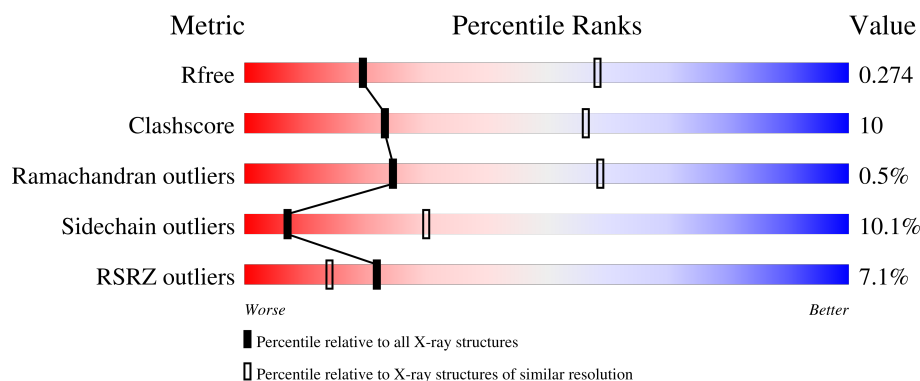
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	761	4% 66% 26% . .
1	B	761	4% 66% 26% . .
1	C	761	11% 67% 25% . .
2	D	20	20% 65% 10% 5% 20%
2	E	20	20% 60% 15% 5% 20%

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Mol	Chain	Length	Quality of chain
2	F	20	
2	P	20	

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
4	GDP	A	763	-	-	-	X
4	GDP	B	763	-	-	-	X
4	GDP	C	763	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18093 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 RIBONUCLEOTIDE REDUCTASE R1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	0	0
			5836	3708	1002	1103	23			
1	B	733	Total	C	N	O	S	0	0	0
			5836	3708	1002	1103	23			
1	C	733	Total	C	N	O	S	0	0	0
			5836	3708	1002	1103	23			

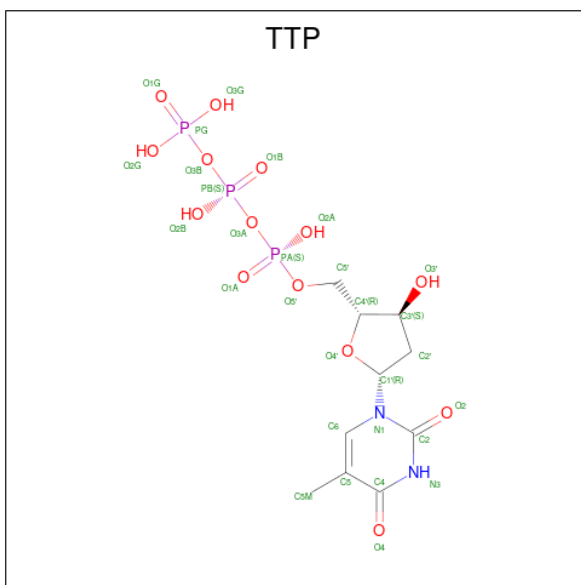
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	ALA	CYS	engineered mutation	UNP P00452
B	292	ALA	CYS	engineered mutation	UNP P00452
C	292	ALA	CYS	engineered mutation	UNP P00452

- Molecule 2 is a protein called RIBONUCLEOTIDE REDUCTASE R2 PROTEIN.

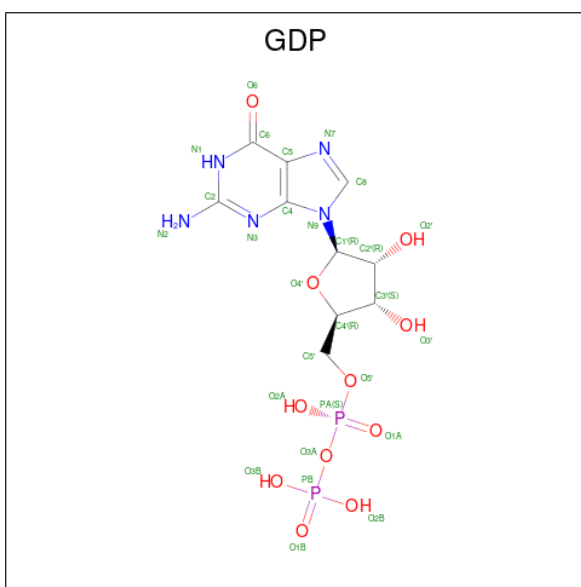
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	E	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	F	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	P	3	Total	C	N	O	0	0	0
			27	20	3	4			

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 29	C 10	N 2	O 14	P 3	0	0
3	B	1	Total 29	C 10	N 2	O 14	P 3	0	0
3	C	1	Total 29	C 10	N 2	O 14	P 3	0	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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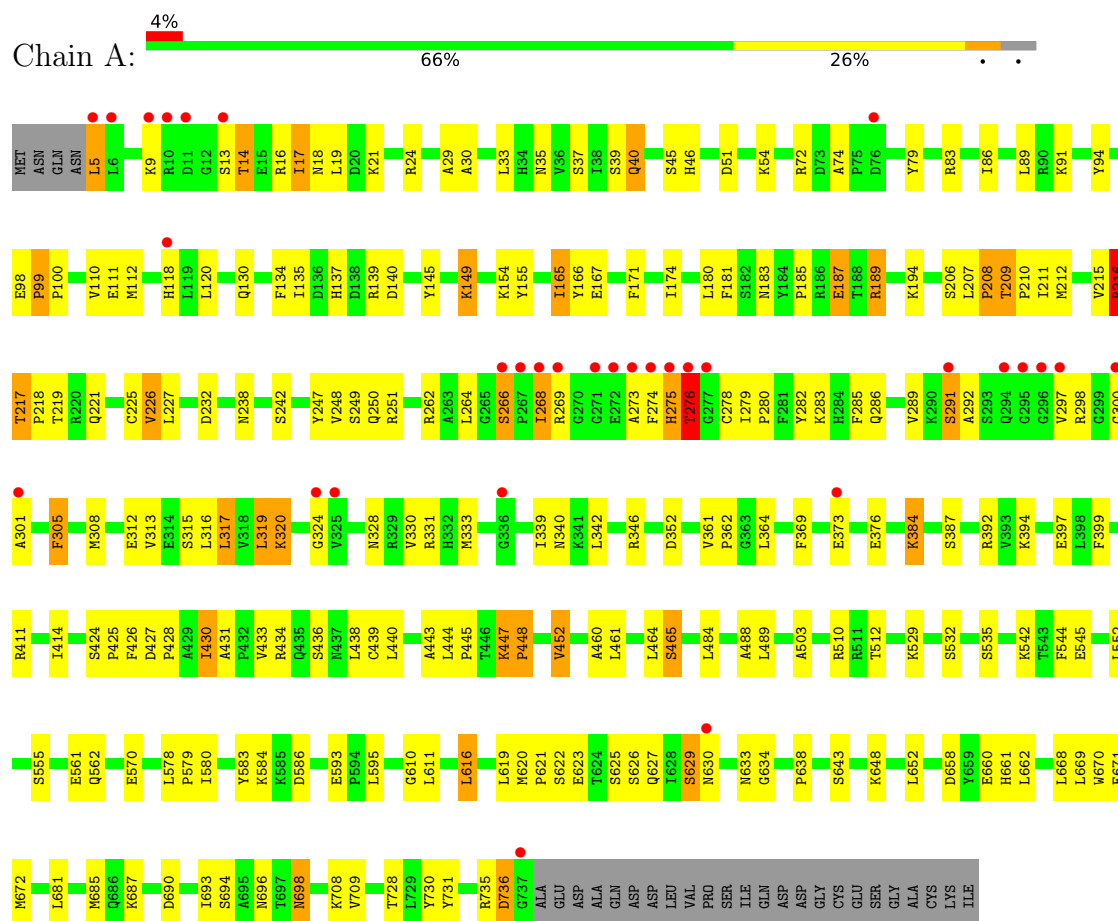
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

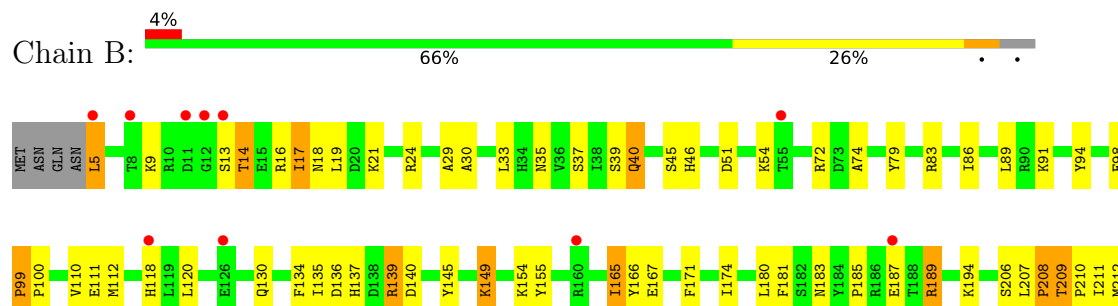
3 Residue-property plots

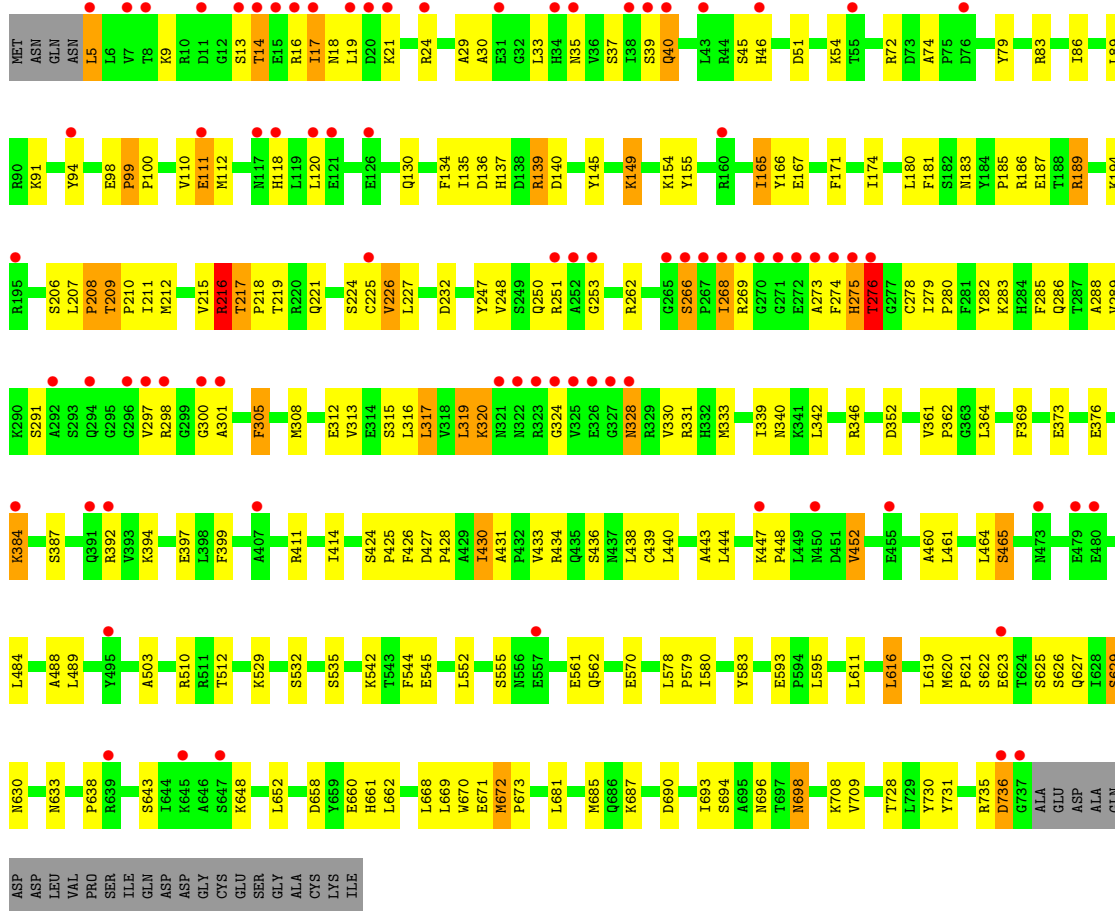
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN



• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

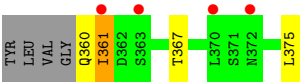




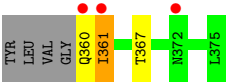
- Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



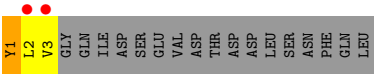
• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	224.02Å 224.02Å 335.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-3.20) 96.8 (20.00-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.01Å)	Xtriage
Refinement program	TNT, REFMAC	Depositor
R, R_{free}	0.278 , 0.308 0.267 , 0.274	Depositor DCC
R_{free} test set	1004 reflections (1.64%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 13.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	18093	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.41	0/5964	1.25	41/8078 (0.5%)
1	B	0.41	0/5964	1.25	41/8078 (0.5%)
1	C	0.41	0/5964	1.25	39/8078 (0.5%)
2	D	0.30	0/129	0.95	0/173
2	E	0.30	0/129	0.95	0/173
2	F	0.30	0/129	0.95	0/173
2	P	0.83	0/27	2.06	1/36 (2.8%)
All	All	0.41	0/18306	1.25	122/24789 (0.5%)

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

There are no bond length outliers.

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	736	ASP	CA-CB-CG	11.05	123.65	112.60
1	B	736	ASP	CA-CB-CG	11.04	123.64	112.60
1	C	736	ASP	CA-CB-CG	11.04	123.64	112.60
1	C	99	PRO	N-CA-CB	10.46	108.66	103.22
1	A	99	PRO	N-CA-CB	10.45	108.65	103.22
1	B	99	PRO	N-CA-CB	10.41	108.64	103.22
1	C	532	SER	N-CA-C	6.76	121.27	112.89
1	A	532	SER	N-CA-C	6.75	121.26	112.89
1	B	532	SER	N-CA-C	6.75	121.25	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	VAL	N-CA-CB	6.63	117.87	110.51
1	A	452	VAL	N-CA-CB	6.60	117.83	110.51
1	C	452	VAL	N-CA-CB	6.60	117.83	110.51
1	B	98	GLU	CA-C-N	6.44	124.30	119.66
1	B	98	GLU	C-N-CA	6.44	124.30	119.66
1	A	98	GLU	CA-C-N	6.43	124.29	119.66
1	A	98	GLU	C-N-CA	6.43	124.29	119.66
1	C	98	GLU	CA-C-N	6.40	124.27	119.66
1	C	98	GLU	C-N-CA	6.40	124.27	119.66
1	B	544	PHE	CA-CB-CG	-6.19	107.61	113.80
1	A	544	PHE	CA-CB-CG	-6.18	107.62	113.80
1	C	544	PHE	CA-CB-CG	-6.16	107.64	113.80
1	A	298	ARG	N-CA-C	6.01	118.44	109.25
1	B	298	ARG	N-CA-C	6.01	118.44	109.25
1	C	298	ARG	N-CA-C	6.00	118.43	109.25
1	B	217	THR	CA-C-N	5.98	125.66	119.56
1	B	217	THR	C-N-CA	5.98	125.66	119.56
1	B	672	MET	CA-C-N	5.96	125.66	119.64
1	B	672	MET	C-N-CA	5.96	125.66	119.64
1	A	217	THR	CA-C-N	5.96	125.64	119.56
1	A	217	THR	C-N-CA	5.96	125.64	119.56
1	C	217	THR	CA-C-N	5.96	125.64	119.56
1	C	217	THR	C-N-CA	5.96	125.64	119.56
1	C	672	MET	CA-C-N	5.94	125.64	119.64
1	C	672	MET	C-N-CA	5.94	125.64	119.64
1	A	672	MET	CA-C-N	5.92	125.62	119.64
1	A	672	MET	C-N-CA	5.92	125.62	119.64
1	C	274	PHE	CA-CB-CG	5.90	119.70	113.80
1	A	274	PHE	CA-CB-CG	5.89	119.69	113.80
1	C	319	LEU	CA-C-O	-5.89	113.45	120.10
1	A	319	LEU	CA-C-O	-5.88	113.45	120.10
1	B	319	LEU	CA-C-O	-5.87	113.47	120.10
1	B	274	PHE	CA-CB-CG	5.86	119.66	113.80
1	B	185	PRO	N-CA-CB	5.76	108.16	103.32
1	A	185	PRO	N-CA-CB	5.72	108.13	103.32
1	C	185	PRO	N-CA-CB	5.69	108.10	103.32
1	B	208	PRO	N-CA-CB	5.61	108.66	103.39
1	B	427	ASP	CA-C-N	5.58	125.42	119.28
1	B	427	ASP	C-N-CA	5.58	125.42	119.28
1	A	208	PRO	N-CA-CB	5.58	108.64	103.39
1	A	427	ASP	CA-C-N	5.58	125.42	119.28
1	A	427	ASP	C-N-CA	5.58	125.42	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	THR	CA-CB-OG1	-5.57	101.24	109.60
1	C	14	THR	N-CA-C	5.56	118.70	109.46
1	C	276	THR	CA-CB-OG1	-5.56	101.25	109.60
1	B	14	THR	N-CA-C	5.56	118.69	109.46
1	B	276	THR	CA-CB-OG1	-5.56	101.27	109.60
1	A	14	THR	N-CA-C	5.55	118.68	109.46
1	C	208	PRO	N-CA-CB	5.55	108.61	103.39
1	C	427	ASP	CA-C-N	5.53	125.36	119.28
1	C	427	ASP	C-N-CA	5.53	125.36	119.28
1	A	305	PHE	CA-CB-CG	-5.50	108.31	113.80
1	C	305	PHE	CA-CB-CG	-5.49	108.31	113.80
1	B	362	PRO	N-CA-CB	5.46	108.10	103.19
1	B	305	PHE	CA-CB-CG	-5.45	108.35	113.80
1	B	690	ASP	CA-CB-CG	-5.44	107.16	112.60
1	A	362	PRO	N-CA-CB	5.42	108.07	103.19
1	C	362	PRO	N-CA-CB	5.39	108.05	103.19
1	A	690	ASP	CA-CB-CG	-5.38	107.22	112.60
1	C	425	PRO	N-CA-CB	5.38	108.31	103.20
1	C	690	ASP	CA-CB-CG	-5.38	107.22	112.60
1	A	425	PRO	N-CA-CB	5.37	108.30	103.20
1	A	331	ARG	N-CA-C	5.35	118.03	111.82
1	B	425	PRO	N-CA-CB	5.35	108.29	103.20
1	A	638	PRO	N-CA-CB	5.33	108.40	103.39
1	C	331	ARG	N-CA-C	5.32	117.99	111.82
1	B	331	ARG	N-CA-C	5.32	117.99	111.82
1	C	638	PRO	N-CA-CB	5.30	108.37	103.39
1	B	638	PRO	N-CA-CB	5.30	108.37	103.39
1	C	276	THR	N-CA-CB	-5.26	102.20	110.46
1	A	276	THR	N-CA-CB	-5.26	102.21	110.46
1	B	276	THR	N-CA-CB	-5.24	102.23	110.46
1	B	430	ILE	CB-CA-C	-5.23	105.54	111.55
1	C	247	TYR	CA-C-O	-5.22	114.89	120.42
1	A	430	ILE	CB-CA-C	-5.20	105.57	111.55
1	C	430	ILE	CB-CA-C	-5.20	105.58	111.55
1	B	74	ALA	CA-C-N	5.19	124.81	119.56
1	B	74	ALA	C-N-CA	5.19	124.81	119.56
1	A	247	TYR	CA-C-O	-5.19	114.92	120.42
1	A	74	ALA	CA-C-N	5.19	124.80	119.56
1	A	74	ALA	C-N-CA	5.19	124.80	119.56
1	B	247	TYR	CA-C-O	-5.18	114.93	120.42
1	B	266	SER	CA-C-N	5.17	124.93	119.76
1	B	266	SER	C-N-CA	5.17	124.93	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	GLY	N-CA-C	5.15	118.10	110.63
1	B	324	GLY	N-CA-C	5.15	118.09	110.63
1	C	74	ALA	CA-C-N	5.14	124.75	119.56
1	C	74	ALA	C-N-CA	5.14	124.75	119.56
1	A	266	SER	CA-C-N	5.14	124.90	119.76
1	A	266	SER	C-N-CA	5.14	124.90	119.76
1	B	448	PRO	N-CA-CB	5.13	107.82	103.35
1	A	448	PRO	N-CA-CB	5.13	107.81	103.35
1	C	448	PRO	N-CA-CB	5.12	107.81	103.35
1	C	324	GLY	N-CA-C	5.12	118.05	110.63
1	C	266	SER	CA-C-N	5.12	124.88	119.76
1	C	266	SER	C-N-CA	5.12	124.88	119.76
1	B	431	ALA	CA-C-N	5.11	125.09	120.03
1	B	431	ALA	C-N-CA	5.11	125.09	120.03
2	P	1	TYR	CA-CB-CG	5.10	123.08	113.90
1	C	593	GLU	CA-C-N	5.10	125.31	120.31
1	C	593	GLU	C-N-CA	5.10	125.31	120.31
1	A	431	ALA	CA-C-N	5.08	125.06	120.03
1	A	431	ALA	C-N-CA	5.08	125.06	120.03
1	A	593	GLU	CA-C-N	5.07	125.28	120.31
1	A	593	GLU	C-N-CA	5.07	125.28	120.31
1	C	431	ALA	CA-C-N	5.07	125.05	120.03
1	C	431	ALA	C-N-CA	5.07	125.05	120.03
1	A	99	PRO	CA-C-N	5.06	125.07	120.21
1	A	99	PRO	C-N-CA	5.06	125.07	120.21
1	B	99	PRO	CA-C-N	5.04	125.05	120.21
1	B	99	PRO	C-N-CA	5.04	125.05	120.21
1	B	593	GLU	CA-C-N	5.01	125.22	120.31
1	B	593	GLU	C-N-CA	5.01	125.22	120.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	ALA	Mainchain

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	5836	0	5764	127	0
1	B	5836	0	5764	122	0
1	C	5836	0	5764	129	0
2	D	129	0	111	1	0
2	E	129	0	111	2	0
2	F	129	0	111	1	0
2	P	27	0	31	10	0
3	A	29	0	13	7	0
3	B	29	0	13	8	0
3	C	29	0	13	7	0
4	A	28	0	12	1	0
4	B	28	0	12	1	0
4	C	28	0	12	1	0
All	All	18093	0	17731	368	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 10.

All (368) 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:A:227:LEU:HB2	1:A:460:ALA:HB3	1.57	0.87
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.57	0.84
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.57	0.84
1:C:120:LEU:HD13	2:P:1:TYR:CG	2.13	0.83
1:C:394:LYS:HB3	1:C:397:GLU:HG3	1.63	0.81
1:B:394:LYS:HB3	1:B:397:GLU:HG3	1.63	0.81
1:C:207:LEU:HB2	1:C:212:MET:HE3	1.64	0.80
1:A:394:LYS:HB3	1:A:397:GLU:HG3	1.63	0.80
1:B:709:VAL:HB	2:E:361:ILE:HG22	1.64	0.80
1:C:215:VAL:O	1:C:216:ARG:HB3	1.82	0.80
1:B:207:LEU:HB2	1:B:212:MET:HE3	1.64	0.80
1:A:215:VAL:O	1:A:216:ARG:HB3	1.82	0.79
1:A:207:LEU:HB2	1:A:212:MET:HE3	1.64	0.79
1:C:709:VAL:HB	2:F:361:ILE:HG22	1.64	0.78
1:A:621:PRO:HD3	1:A:694:SER:OG	1.84	0.78
1:B:621:PRO:HD3	1:B:694:SER:OG	1.84	0.78
1:B:215:VAL:O	1:B:216:ARG:HB3	1.82	0.78
1:C:621:PRO:HD3	1:C:694:SER:OG	1.84	0.77
1:A:709:VAL:HB	2:D:361:ILE:HG22	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ASP:HB3	1:C:662:LEU:HD12	1.70	0.73
1:A:658:ASP:HB3	1:A:662:LEU:HD12	1.70	0.73
1:B:658:ASP:HB3	1:B:662:LEU:HD12	1.70	0.73
1:A:268:ILE:HB	1:A:273:ALA:HB3	1.71	0.72
1:B:268:ILE:HB	1:B:273:ALA:HB3	1.72	0.71
1:A:149:LYS:HG2	1:A:652:LEU:HD21	1.73	0.71
1:C:268:ILE:HB	1:C:273:ALA:HB3	1.71	0.70
1:C:320:LYS:HE2	1:C:411:ARG:HB2	1.74	0.70
1:A:320:LYS:HE2	1:A:411:ARG:HB2	1.74	0.70
1:B:320:LYS:HE2	1:B:411:ARG:HB2	1.73	0.70
1:C:149:LYS:HG2	1:C:652:LEU:HD21	1.73	0.70
1:B:149:LYS:HG2	1:B:652:LEU:HD21	1.73	0.69
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.76	0.68
1:A:155:TYR:HE1	1:A:209:THR:HG23	1.59	0.67
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.75	0.67
1:B:155:TYR:HE1	1:B:209:THR:HG23	1.59	0.67
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.75	0.67
1:C:155:TYR:HE1	1:C:209:THR:HG23	1.59	0.67
1:B:430:ILE:HG21	1:B:570:GLU:HG2	1.76	0.66
1:C:430:ILE:HG21	1:C:570:GLU:HG2	1.76	0.66
1:A:430:ILE:HG21	1:A:570:GLU:HG2	1.76	0.65
1:A:313:VAL:HG22	1:A:317:LEU:HD22	1.79	0.65
1:A:439:CYS:HA	1:A:730:TYR:CE1	2.33	0.64
1:B:313:VAL:HG22	1:B:317:LEU:HD22	1.79	0.63
1:C:111:GLU:OE2	2:P:2:LEU:N	2.31	0.63
1:C:313:VAL:HG22	1:C:317:LEU:HD22	1.79	0.63
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.81	0.62
1:C:439:CYS:HA	1:C:730:TYR:CE1	2.33	0.62
1:B:439:CYS:HA	1:B:730:TYR:CE1	2.33	0.62
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.81	0.62
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.81	0.62
1:A:276:THR:HG23	1:B:293:SER:O	2.01	0.60
1:C:250:GLN:O	1:C:251:ARG:HB2	2.01	0.60
1:A:79:TYR:O	1:A:83:ARG:HG3	2.01	0.60
1:B:79:TYR:O	1:B:83:ARG:HG3	2.01	0.60
1:C:620:MET:HG2	1:C:621:PRO:O	2.02	0.60
1:A:250:GLN:O	1:A:251:ARG:HB2	2.01	0.60
1:A:342:LEU:HD13	1:A:376:GLU:HG3	1.83	0.60
1:B:250:GLN:O	1:B:251:ARG:HB2	2.01	0.60
1:A:275:HIS:CD2	3:A:762:TTP:H1'	2.36	0.60
1:C:79:TYR:O	1:C:83:ARG:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:HIS:CD2	3:B:762:TTP:H1'	2.36	0.60
1:C:342:LEU:HD13	1:C:376:GLU:HG3	1.83	0.60
1:B:342:LEU:HD13	1:B:376:GLU:HG3	1.83	0.59
1:A:620:MET:HG2	1:A:621:PRO:O	2.02	0.59
1:B:620:MET:HG2	1:B:621:PRO:O	2.02	0.59
1:C:275:HIS:CD2	3:C:762:TTP:H1'	2.36	0.59
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.85	0.59
1:A:268:ILE:HD13	3:A:762:TTP:C4	2.38	0.59
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.85	0.58
1:B:268:ILE:HG21	3:B:762:TTP:C5	2.38	0.58
1:A:268:ILE:HD11	1:A:275:HIS:HA	1.86	0.58
1:A:248:VAL:HG11	1:A:289:VAL:HA	1.86	0.58
1:B:248:VAL:HG11	1:B:289:VAL:HA	1.86	0.58
1:C:111:GLU:HG3	2:P:2:LEU:O	2.04	0.58
1:C:248:VAL:HG11	1:C:289:VAL:HA	1.86	0.58
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.85	0.58
1:A:268:ILE:HG21	3:A:762:TTP:C5	2.38	0.58
1:B:268:ILE:HD13	3:B:762:TTP:C4	2.38	0.58
1:C:268:ILE:HG21	3:C:762:TTP:C5	2.38	0.58
1:B:232:ASP:OD1	1:B:262:ARG:HG2	2.04	0.58
1:C:232:ASP:OD1	1:C:262:ARG:HG2	2.04	0.58
1:C:268:ILE:HD13	3:C:762:TTP:C4	2.38	0.58
1:A:384:LYS:NZ	1:A:392:ARG:HH22	2.02	0.57
1:B:384:LYS:NZ	1:B:392:ARG:HH22	2.02	0.57
1:C:384:LYS:NZ	1:C:392:ARG:HH22	2.02	0.57
1:A:232:ASP:OD1	1:A:262:ARG:HG2	2.04	0.57
1:C:268:ILE:HD11	1:C:275:HIS:HA	1.86	0.57
1:A:291:SER:O	1:B:276:THR:HG21	2.05	0.56
1:B:268:ILE:HD11	1:B:275:HIS:HA	1.86	0.56
1:C:279:ILE:HD12	1:C:319:LEU:HD21	1.87	0.56
1:C:110:VAL:HG11	1:C:120:LEU:HD12	1.87	0.56
1:A:279:ILE:HD12	1:A:319:LEU:HD21	1.87	0.56
1:B:110:VAL:HG11	1:B:120:LEU:HD12	1.87	0.56
1:B:279:ILE:HD12	1:B:319:LEU:HD21	1.87	0.56
1:A:268:ILE:HG21	3:A:762:TTP:C6	2.41	0.56
1:C:555:SER:HB3	1:C:611:LEU:HD22	1.88	0.56
1:A:110:VAL:HG11	1:A:120:LEU:HD12	1.87	0.55
1:B:268:ILE:HG21	3:B:762:TTP:C6	2.41	0.55
1:B:555:SER:HB3	1:B:611:LEU:HD22	1.88	0.55
1:A:276:THR:HG22	1:A:280:PRO:HG2	1.88	0.55
1:A:555:SER:HB3	1:A:611:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LEU:HD13	2:P:1:TYR:CB	2.36	0.55
1:A:268:ILE:HD13	3:A:762:TTP:N3	2.22	0.55
1:C:268:ILE:HG21	3:C:762:TTP:C6	2.40	0.55
1:C:276:THR:HG22	1:C:280:PRO:HG2	1.88	0.55
1:B:465:SER:HB2	1:B:489:LEU:HD11	1.89	0.54
1:A:99:PRO:HG2	1:A:137:HIS:CD2	2.42	0.54
1:B:346:ARG:HD2	1:B:352:ASP:O	2.08	0.54
1:B:268:ILE:HD13	3:B:762:TTP:N3	2.22	0.54
1:C:268:ILE:HD13	3:C:762:TTP:N3	2.22	0.54
1:B:276:THR:HG22	1:B:280:PRO:HG2	1.88	0.54
1:A:346:ARG:HD2	1:A:352:ASP:O	2.08	0.54
1:B:99:PRO:HG2	1:B:137:HIS:CD2	2.42	0.54
1:C:346:ARG:HD2	1:C:352:ASP:O	2.08	0.54
1:A:187:GLU:CD	1:C:186:ARG:NH1	2.66	0.54
1:C:99:PRO:HG2	1:C:137:HIS:CD2	2.42	0.53
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.90	0.53
1:C:111:GLU:CG	2:P:2:LEU:HB2	2.38	0.53
1:C:622:SER:O	1:C:633:ASN:HB3	2.08	0.53
1:C:555:SER:HB2	1:C:616:LEU:HD21	1.90	0.53
1:C:465:SER:HB2	1:C:489:LEU:HD11	1.89	0.53
1:A:264:LEU:HD11	1:B:294:GLN:NE2	2.24	0.53
1:B:555:SER:HB2	1:B:616:LEU:HD21	1.90	0.53
1:A:5:LEU:O	1:A:17:ILE:HB	2.09	0.53
1:A:622:SER:O	1:A:633:ASN:HB3	2.08	0.52
1:A:555:SER:HB2	1:A:616:LEU:HD21	1.90	0.52
1:A:268:ILE:O	1:A:269:ARG:HB3	2.10	0.52
1:B:622:SER:O	1:B:633:ASN:HB3	2.08	0.52
1:A:187:GLU:OE1	1:C:186:ARG:HG3	2.10	0.52
1:A:249:SER:HB2	3:B:762:TTP:C4	2.45	0.52
1:B:5:LEU:O	1:B:17:ILE:HB	2.09	0.52
1:A:529:LYS:HD2	1:A:535:SER:O	2.10	0.52
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.92	0.52
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.92	0.52
1:B:37:SER:OG	1:B:40:GLN:HB2	2.10	0.52
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.92	0.52
1:C:5:LEU:O	1:C:17:ILE:HB	2.09	0.52
1:A:37:SER:OG	1:A:40:GLN:HB2	2.10	0.51
1:B:561:GLU:HG2	1:B:562:GLN:HG3	1.92	0.51
1:B:268:ILE:O	1:B:269:ARG:HB3	2.10	0.51
1:C:120:LEU:HD13	2:P:1:TYR:CD2	2.45	0.51
1:C:37:SER:OG	1:C:40:GLN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:PHE:CG	1:A:434:ARG:HG2	2.46	0.51
1:B:529:LYS:HD2	1:B:535:SER:O	2.10	0.51
1:C:268:ILE:O	1:C:269:ARG:HB3	2.10	0.51
1:C:668:LEU:HB2	1:C:671:GLU:HG3	1.93	0.51
1:B:668:LEU:HB2	1:B:671:GLU:HG3	1.93	0.51
3:A:762:TTP:C4	1:B:249:SER:HB2	2.46	0.50
1:B:369:PHE:CG	1:B:434:ARG:HG2	2.45	0.50
1:C:369:PHE:CG	1:C:434:ARG:HG2	2.45	0.50
1:C:529:LYS:HD2	1:C:535:SER:O	2.10	0.50
1:A:561:GLU:HG2	1:A:562:GLN:HG3	1.92	0.50
1:B:167:GLU:OE2	1:B:216:ARG:NH1	2.45	0.50
1:B:510:ARG:NH2	1:B:570:GLU:OE1	2.45	0.50
1:C:670:TRP:CE2	1:C:735:ARG:HG3	2.47	0.50
1:A:610:GLY:HA3	2:P:2:LEU:CD2	2.42	0.50
1:A:668:LEU:HB2	1:A:671:GLU:HG3	1.93	0.50
1:A:670:TRP:CE2	1:A:735:ARG:HG3	2.47	0.50
1:B:670:TRP:CE2	1:B:735:ARG:HG3	2.47	0.50
1:C:561:GLU:HG2	1:C:562:GLN:HG3	1.92	0.50
1:C:167:GLU:OE2	1:C:216:ARG:NH1	2.45	0.49
1:C:510:ARG:NH2	1:C:570:GLU:OE1	2.45	0.49
1:A:207:LEU:HD23	1:A:465:SER:OG	2.13	0.49
1:A:217:THR:OG1	1:A:219:THR:HG22	2.12	0.49
1:C:312:GLU:O	1:C:316:LEU:HG	2.13	0.49
1:C:207:LEU:HD23	1:C:465:SER:OG	2.13	0.49
1:A:276:THR:CG2	1:A:280:PRO:HG2	2.43	0.49
1:A:30:ALA:HA	1:A:33:LEU:HD12	1.94	0.49
1:A:209:THR:N	1:A:210:PRO:HD2	2.28	0.49
1:A:510:ARG:NH2	1:A:570:GLU:OE1	2.45	0.49
1:C:217:THR:OG1	1:C:219:THR:HG22	2.12	0.49
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.94	0.49
1:B:207:LEU:HD23	1:B:465:SER:OG	2.13	0.49
1:B:217:THR:OG1	1:B:219:THR:HG22	2.12	0.49
1:B:312:GLU:O	1:B:316:LEU:HG	2.13	0.49
1:B:209:THR:N	1:B:210:PRO:HD2	2.28	0.49
1:C:30:ALA:HA	1:C:33:LEU:HD12	1.94	0.49
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.94	0.48
1:A:167:GLU:OE2	1:A:216:ARG:NH1	2.45	0.48
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.94	0.48
1:A:187:GLU:OE2	1:C:186:ARG:NH1	2.46	0.48
1:C:461:LEU:HD11	1:C:503:ALA:HB1	1.96	0.48
1:A:312:GLU:O	1:A:316:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:PHE:O	1:C:289:VAL:HG23	2.14	0.48
1:B:285:PHE:O	1:B:289:VAL:HG23	2.14	0.48
1:B:583:TYR:CD2	1:B:687:LYS:HD2	2.48	0.48
1:C:583:TYR:CD2	1:C:687:LYS:HD2	2.48	0.48
1:A:285:PHE:O	1:A:289:VAL:HG23	2.14	0.48
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.95	0.48
1:C:209:THR:N	1:C:210:PRO:HD2	2.28	0.48
1:A:17:ILE:HD13	1:A:18:ASN:N	2.29	0.48
1:A:583:TYR:CD2	1:A:687:LYS:HD2	2.48	0.48
1:B:112:MET:HE1	1:B:166:TYR:CE1	2.49	0.48
1:B:276:THR:CG2	1:B:280:PRO:HG2	2.43	0.48
1:C:112:MET:HE1	1:C:166:TYR:CE1	2.49	0.48
1:C:217:THR:HB	1:C:218:PRO:HD2	1.96	0.48
1:B:224:SER:O	1:B:253:GLY:N	2.41	0.47
1:A:212:MET:O	1:A:216:ARG:NH2	2.47	0.47
1:B:217:THR:HB	1:B:218:PRO:HD2	1.96	0.47
1:B:552:LEU:HD23	1:B:616:LEU:HD13	1.96	0.47
1:A:112:MET:HE1	1:A:166:TYR:CE1	2.49	0.47
1:B:461:LEU:HD11	1:B:503:ALA:HB1	1.96	0.47
1:C:111:GLU:CD	2:P:2:LEU:HB2	2.39	0.47
1:C:212:MET:O	1:C:216:ARG:NH2	2.47	0.47
1:C:276:THR:CG2	1:C:280:PRO:HG2	2.43	0.47
1:A:134:PHE:CG	1:A:194:LYS:HG3	2.50	0.47
1:A:552:LEU:HD23	1:A:616:LEU:HD13	1.96	0.47
1:A:268:ILE:HD12	1:A:273:ALA:HB1	1.96	0.47
1:A:464:LEU:HB3	1:A:620:MET:HE2	1.96	0.47
1:B:5:LEU:HD22	1:B:17:ILE:HG13	1.97	0.47
1:B:134:PHE:CG	1:B:194:LYS:HG3	2.50	0.47
1:B:268:ILE:HD12	1:B:273:ALA:HB1	1.96	0.47
1:C:5:LEU:HD22	1:C:17:ILE:HG13	1.97	0.47
1:C:17:ILE:HD13	1:C:18:ASN:N	2.29	0.47
1:C:134:PHE:CG	1:C:194:LYS:HG3	2.50	0.47
1:A:461:LEU:HD11	1:A:503:ALA:HB1	1.96	0.47
1:B:17:ILE:HD13	1:B:18:ASN:N	2.29	0.47
1:B:464:LEU:HB3	1:B:620:MET:HE2	1.96	0.47
1:C:224:SER:O	1:C:253:GLY:N	2.40	0.47
1:B:181:PHE:O	1:B:189:ARG:HD2	2.15	0.46
1:A:29:ALA:O	1:A:83:ARG:HD2	2.15	0.46
1:B:212:MET:O	1:B:216:ARG:NH2	2.47	0.46
1:A:181:PHE:O	1:A:189:ARG:HD2	2.15	0.46
1:C:181:PHE:O	1:C:189:ARG:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:GLY:HA3	2:P:2:LEU:HD23	1.97	0.46
1:B:29:ALA:O	1:B:83:ARG:HD2	2.15	0.46
1:C:29:ALA:O	1:C:83:ARG:HD2	2.15	0.46
1:C:552:LEU:HD23	1:C:616:LEU:HD13	1.96	0.46
1:C:268:ILE:HD12	1:C:273:ALA:HB1	1.96	0.46
1:A:5:LEU:HD22	1:A:17:ILE:HG13	1.97	0.46
1:A:217:THR:HB	1:A:218:PRO:HD2	1.96	0.46
1:C:464:LEU:HB3	1:C:620:MET:HE2	1.96	0.46
1:A:208:PRO:HB2	1:A:210:PRO:HD2	1.98	0.45
1:A:171:PHE:HA	1:A:174:ILE:HG22	1.98	0.45
1:C:171:PHE:HA	1:C:174:ILE:HG22	1.98	0.45
1:A:276:THR:HG21	1:B:293:SER:H	1.82	0.45
1:B:660:GLU:HB3	1:B:661:HIS:HD2	1.82	0.45
1:C:660:GLU:HB3	1:C:661:HIS:HD2	1.82	0.45
1:C:208:PRO:HB2	1:C:210:PRO:HD2	1.98	0.45
1:A:660:GLU:HB3	1:A:661:HIS:HD2	1.82	0.44
1:B:180:LEU:CD1	1:B:488:ALA:HB1	2.48	0.44
1:B:226:VAL:HA	1:B:460:ALA:O	2.17	0.44
1:B:262:ARG:HG3	1:B:275:HIS:CD2	2.52	0.44
1:C:18:ASN:ND2	1:C:21:LYS:HG3	2.32	0.44
1:B:208:PRO:HB2	1:B:210:PRO:HD2	1.98	0.44
1:A:440:LEU:HD12	1:A:728:THR:HB	1.98	0.44
1:C:262:ARG:HG3	1:C:275:HIS:CD2	2.52	0.44
1:B:19:LEU:HD22	1:B:46:HIS:CE1	2.53	0.44
1:B:440:LEU:HD12	1:B:728:THR:HB	1.98	0.44
1:B:629:SER:O	1:B:630:ASN:C	2.61	0.44
1:C:19:LEU:HD22	1:C:46:HIS:CE1	2.53	0.44
1:A:18:ASN:ND2	1:A:21:LYS:HG3	2.32	0.44
1:A:301:ALA:HB3	1:A:438:LEU:CD2	2.48	0.44
1:B:301:ALA:HB3	1:B:438:LEU:CD2	2.48	0.44
1:C:226:VAL:HA	1:C:460:ALA:O	2.18	0.44
1:C:623:GLU:O	1:C:627:GLN:HG3	2.17	0.44
1:A:145:TYR:CZ	1:A:149:LYS:HD3	2.53	0.44
1:A:238:ASN:HB3	1:B:242:SER:OG	2.17	0.44
1:A:275:HIS:HE2	3:A:762:TTP:H2'1	1.83	0.44
1:C:111:GLU:CD	2:P:2:LEU:HD12	2.42	0.44
1:C:145:TYR:CZ	1:C:149:LYS:HD3	2.53	0.44
1:C:275:HIS:HE2	3:C:762:TTP:H2'1	1.83	0.44
1:C:301:ALA:HB3	1:C:438:LEU:CD2	2.48	0.44
1:C:440:LEU:HD12	1:C:728:THR:HB	1.98	0.44
1:B:275:HIS:HE2	3:B:762:TTP:H2'1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:HG3	1:A:275:HIS:CD2	2.52	0.44
1:A:623:GLU:O	1:A:627:GLN:HG3	2.18	0.44
1:B:18:ASN:ND2	1:B:21:LYS:HG3	2.32	0.44
1:B:171:PHE:HA	1:B:174:ILE:HG22	1.98	0.43
1:C:180:LEU:CD1	1:C:488:ALA:HB1	2.48	0.43
1:A:384:LYS:HZ2	1:A:392:ARG:HH22	1.63	0.43
1:B:208:PRO:HD2	1:B:211:ILE:HD12	2.00	0.43
1:C:328:ASN:HD22	1:C:328:ASN:HA	1.64	0.43
1:A:180:LEU:CD1	1:A:488:ALA:HB1	2.48	0.43
1:B:145:TYR:CZ	1:B:149:LYS:HD3	2.52	0.43
1:B:623:GLU:O	1:B:627:GLN:HG3	2.18	0.43
1:B:669:LEU:HD11	1:B:698:ASN:CG	2.43	0.43
1:C:672:MET:HA	1:C:673:PRO:HD3	1.80	0.43
1:C:208:PRO:HD2	1:C:211:ILE:HD12	2.00	0.43
1:A:226:VAL:HA	1:A:460:ALA:O	2.17	0.43
1:A:669:LEU:HD11	1:A:698:ASN:CG	2.43	0.43
1:B:339:ILE:HG22	1:B:340:ASN:N	2.34	0.43
1:A:221:GLN:OE1	1:A:250:GLN:HG2	2.19	0.43
1:A:447:LYS:HA	1:A:448:PRO:HD3	1.90	0.43
1:A:629:SER:O	1:A:630:ASN:C	2.61	0.43
1:B:584:LYS:NZ	2:E:375:LEU:O	2.46	0.43
1:C:669:LEU:HD11	1:C:698:ASN:CG	2.43	0.43
1:A:19:LEU:HD22	1:A:46:HIS:CE1	2.53	0.43
1:A:426:PHE:O	1:A:428:PRO:HD3	2.19	0.43
1:B:426:PHE:O	1:B:428:PRO:HD3	2.19	0.43
1:A:208:PRO:HD2	1:A:211:ILE:HD12	2.00	0.43
1:A:283:LYS:CG	1:A:330:VAL:HG22	2.49	0.43
1:B:86:ILE:HG21	1:B:140:ASP:HB3	2.01	0.43
1:B:369:PHE:CD1	1:B:434:ARG:HA	2.54	0.43
1:C:86:ILE:HG21	1:C:140:ASP:HB3	2.01	0.43
1:C:369:PHE:CD1	1:C:434:ARG:HA	2.54	0.43
1:C:629:SER:O	1:C:630:ASN:C	2.61	0.43
1:A:369:PHE:CD1	1:A:434:ARG:HA	2.54	0.42
1:C:339:ILE:HG22	1:C:340:ASN:N	2.34	0.42
1:C:320:LYS:HE2	1:C:411:ARG:CB	2.47	0.42
1:A:89:LEU:CD2	1:A:165:ILE:HD13	2.50	0.42
1:A:94:TYR:CG	1:A:100:PRO:HD3	2.54	0.42
1:B:320:LYS:HE2	1:B:411:ARG:CB	2.47	0.42
1:C:283:LYS:CG	1:C:330:VAL:HG22	2.49	0.42
1:C:94:TYR:CG	1:C:100:PRO:HD3	2.54	0.42
1:C:221:GLN:OE1	1:C:250:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:LYS:NZ	1:A:586:ASP:OD1	2.52	0.42
1:B:221:GLN:OE1	1:B:250:GLN:HG2	2.19	0.42
1:C:286:GLN:HG3	1:C:333:MET:HG3	2.02	0.42
1:A:320:LYS:HE2	1:A:411:ARG:CB	2.47	0.42
1:A:545:GLU:HG3	1:A:595:LEU:HD23	2.02	0.42
1:B:545:GLU:HG3	1:B:595:LEU:HD23	2.02	0.42
1:B:286:GLN:HG3	1:B:333:MET:HG3	2.01	0.42
1:A:286:GLN:HG3	1:A:333:MET:HG3	2.01	0.42
1:B:439:CYS:SG	4:B:763:GDP:H3'	2.60	0.42
1:A:578:LEU:HB3	1:A:579:PRO:HD2	2.02	0.42
1:B:283:LYS:CG	1:B:330:VAL:HG22	2.49	0.42
1:A:86:ILE:HG21	1:A:140:ASP:HB3	2.01	0.41
1:A:339:ILE:HG22	1:A:340:ASN:N	2.34	0.41
1:A:439:CYS:SG	4:A:763:GDP:H3'	2.60	0.41
1:C:89:LEU:CD2	1:C:165:ILE:HD13	2.50	0.41
1:C:426:PHE:O	1:C:428:PRO:HD3	2.19	0.41
1:C:545:GLU:HG3	1:C:595:LEU:HD23	2.02	0.41
1:B:94:TYR:CG	1:B:100:PRO:HD3	2.54	0.41
1:B:94:TYR:CD1	1:B:100:PRO:HD3	2.55	0.41
1:C:136:ASP:HB3	1:C:139:ARG:HG3	2.02	0.41
1:A:384:LYS:HZ2	1:A:392:ARG:NH2	2.17	0.41
1:A:444:LEU:HA	1:A:445:PRO:HD3	1.92	0.41
1:B:578:LEU:HB3	1:B:579:PRO:HD2	2.02	0.41
1:C:94:TYR:CD1	1:C:100:PRO:HD3	2.56	0.41
1:C:439:CYS:SG	4:C:763:GDP:H3'	2.60	0.41
1:B:89:LEU:CD2	1:B:165:ILE:HD13	2.50	0.41
1:B:282:TYR:CE2	1:B:316:LEU:HD22	2.56	0.41
1:C:282:TYR:CE2	1:C:316:LEU:HD22	2.56	0.41
1:C:578:LEU:HB3	1:C:579:PRO:HD2	2.02	0.41
1:A:242:SER:OG	1:B:238:ASN:HB3	2.20	0.41
1:B:136:ASP:HB3	1:B:139:ARG:HG3	2.02	0.41
1:B:305:PHE:CZ	1:B:436:SER:HB3	2.56	0.41
1:A:681:LEU:O	1:A:685:MET:HG3	2.20	0.41
1:C:305:PHE:CZ	1:C:436:SER:HB3	2.56	0.41
1:A:94:TYR:CD1	1:A:100:PRO:HD3	2.56	0.41
1:A:305:PHE:CZ	1:A:436:SER:HB3	2.56	0.41
1:B:384:LYS:HZ1	1:B:392:ARG:HH22	1.67	0.41
1:C:681:LEU:O	1:C:685:MET:HG3	2.20	0.41
1:A:283:LYS:HG3	1:A:330:VAL:HG22	2.03	0.41
1:B:248:VAL:HG21	1:B:288:ALA:O	2.21	0.41
1:B:308:MET:HE1	1:B:399:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:VAL:O	1:C:216:ARG:CB	2.59	0.41
1:C:248:VAL:HG21	1:C:288:ALA:O	2.21	0.41
1:C:308:MET:HE1	1:C:399:PHE:CZ	2.56	0.41
1:B:269:ARG:O	1:B:269:ARG:HG3	2.21	0.41
1:B:681:LEU:O	1:B:685:MET:HG3	2.20	0.41
1:A:308:MET:HE1	1:A:399:PHE:CZ	2.56	0.40
1:C:275:HIS:NE2	3:C:762:TTP:H2'1	2.37	0.40
1:A:264:LEU:HD11	1:B:294:GLN:HE22	1.87	0.40
1:C:155:TYR:CE1	1:C:209:THR:HG23	2.49	0.40
1:C:278:CYS:HB3	1:C:282:TYR:CE1	2.56	0.40
1:C:283:LYS:HG3	1:C:330:VAL:HG22	2.03	0.40
1:C:621:PRO:HD3	1:C:694:SER:CB	2.52	0.40
1:A:209:THR:N	1:A:210:PRO:CD	2.85	0.40
1:A:633:ASN:O	1:A:634:GLY:C	2.64	0.40
1:C:583:TYR:CG	1:C:687:LYS:HD2	2.56	0.40
1:A:278:CYS:O	1:A:279:ILE:C	2.65	0.40
1:A:282:TYR:CE2	1:A:316:LEU:HD22	2.56	0.40
1:B:275:HIS:NE2	3:B:762:TTP:H2'1	2.37	0.40
1:B:278:CYS:HB3	1:B:282:TYR:CE1	2.56	0.40
1:B:283:LYS:HG3	1:B:330:VAL:HG22	2.03	0.40
1:C:384:LYS:HZ2	1:C:392:ARG:HH22	1.68	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	731/761 (96%)	694 (95%)	33 (4%)	4 (0%)	24	59
1	B	731/761 (96%)	694 (95%)	33 (4%)	4 (0%)	24	59
1	C	731/761 (96%)	694 (95%)	33 (4%)	4 (0%)	24	59
2	D	14/20 (70%)	13 (93%)	1 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	F	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	P	1/20 (5%)	1 (100%)	0	0	100	100
All	All	2236/2363 (95%)	2122 (95%)	102 (5%)	12 (0%)	24	59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	HIS
1	B	275	HIS
1	C	275	HIS
1	A	216	ARG
1	B	216	ARG
1	C	216	ARG
1	A	300	GLY
1	B	300	GLY
1	C	300	GLY
1	A	731	TYR
1	B	731	TYR
1	C	731	TYR

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	627/650 (96%)	565 (90%)	62 (10%)	7	31
1	B	627/650 (96%)	565 (90%)	62 (10%)	7	31
1	C	627/650 (96%)	565 (90%)	62 (10%)	7	31
2	D	16/19 (84%)	13 (81%)	3 (19%)	1	9
2	E	16/19 (84%)	13 (81%)	3 (19%)	1	9
2	F	16/19 (84%)	13 (81%)	3 (19%)	1	9
2	P	3/19 (16%)	2 (67%)	1 (33%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1932/2026 (95%)	1736 (90%)	196 (10%)	7 30

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	LYS
1	A	13	SER
1	A	14	THR
1	A	16	ARG
1	A	17	ILE
1	A	24	ARG
1	A	35	ASN
1	A	39	SER
1	A	40	GLN
1	A	45	SER
1	A	51	ASP
1	A	54	LYS
1	A	72	ARG
1	A	91	LYS
1	A	111	GLU
1	A	118	HIS
1	A	130	GLN
1	A	139	ARG
1	A	149	LYS
1	A	154	LYS
1	A	165	ILE
1	A	183	ASN
1	A	187	GLU
1	A	189	ARG
1	A	206	SER
1	A	209	THR
1	A	216	ARG
1	A	225	CYS
1	A	226	VAL
1	A	266	SER
1	A	268	ILE
1	A	276	THR
1	A	291	SER
1	A	297	VAL
1	A	315	SER
1	A	317	LEU

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Mol	Chain	Res	Type
1	A	320	LYS
1	A	328	ASN
1	A	361	VAL
1	A	364	LEU
1	A	373	GLU
1	A	384	LYS
1	A	387	SER
1	A	414	ILE
1	A	424	SER
1	A	447	LYS
1	A	452	VAL
1	A	465	SER
1	A	484	LEU
1	A	542	LYS
1	A	580	ILE
1	A	616	LEU
1	A	625	SER
1	A	626	SER
1	A	629	SER
1	A	643	SER
1	A	648	LYS
1	A	696	ASN
1	A	698	ASN
1	A	708	LYS
1	A	736	ASP
2	D	360	GLN
2	D	361	ILE
2	D	367	THR
1	B	5	LEU
1	B	9	LYS
1	B	13	SER
1	B	14	THR
1	B	16	ARG
1	B	17	ILE
1	B	24	ARG
1	B	35	ASN
1	B	39	SER
1	B	40	GLN
1	B	45	SER
1	B	51	ASP
1	B	54	LYS
1	B	72	ARG

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Mol	Chain	Res	Type
1	B	91	LYS
1	B	111	GLU
1	B	118	HIS
1	B	130	GLN
1	B	139	ARG
1	B	149	LYS
1	B	154	LYS
1	B	165	ILE
1	B	183	ASN
1	B	187	GLU
1	B	189	ARG
1	B	206	SER
1	B	209	THR
1	B	216	ARG
1	B	225	CYS
1	B	226	VAL
1	B	266	SER
1	B	268	ILE
1	B	276	THR
1	B	291	SER
1	B	297	VAL
1	B	315	SER
1	B	317	LEU
1	B	320	LYS
1	B	328	ASN
1	B	361	VAL
1	B	364	LEU
1	B	373	GLU
1	B	384	LYS
1	B	387	SER
1	B	414	ILE
1	B	424	SER
1	B	447	LYS
1	B	452	VAL
1	B	465	SER
1	B	484	LEU
1	B	542	LYS
1	B	580	ILE
1	B	616	LEU
1	B	625	SER
1	B	626	SER
1	B	629	SER

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Mol	Chain	Res	Type
1	B	643	SER
1	B	648	LYS
1	B	696	ASN
1	B	698	ASN
1	B	708	LYS
1	B	736	ASP
2	E	360	GLN
2	E	361	ILE
2	E	367	THR
1	C	5	LEU
1	C	9	LYS
1	C	13	SER
1	C	14	THR
1	C	16	ARG
1	C	17	ILE
1	C	24	ARG
1	C	35	ASN
1	C	39	SER
1	C	40	GLN
1	C	45	SER
1	C	51	ASP
1	C	54	LYS
1	C	72	ARG
1	C	91	LYS
1	C	111	GLU
1	C	118	HIS
1	C	130	GLN
1	C	139	ARG
1	C	149	LYS
1	C	154	LYS
1	C	165	ILE
1	C	183	ASN
1	C	187	GLU
1	C	189	ARG
1	C	206	SER
1	C	209	THR
1	C	216	ARG
1	C	225	CYS
1	C	226	VAL
1	C	266	SER
1	C	268	ILE
1	C	276	THR

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Mol	Chain	Res	Type
1	C	291	SER
1	C	297	VAL
1	C	315	SER
1	C	317	LEU
1	C	320	LYS
1	C	328	ASN
1	C	361	VAL
1	C	364	LEU
1	C	373	GLU
1	C	384	LYS
1	C	387	SER
1	C	414	ILE
1	C	424	SER
1	C	447	LYS
1	C	452	VAL
1	C	465	SER
1	C	484	LEU
1	C	542	LYS
1	C	580	ILE
1	C	616	LEU
1	C	625	SER
1	C	626	SER
1	C	629	SER
1	C	643	SER
1	C	648	LYS
1	C	696	ASN
1	C	698	ASN
1	C	708	LYS
1	C	736	ASP
2	F	360	GLN
2	F	361	ILE
2	F	367	THR
2	P	3	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	250	GLN
1	A	328	ASN
1	A	332	HIS
1	A	661	HIS

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Mol	Chain	Res	Type
1	A	696	ASN
1	A	733	ASN
2	D	360	GLN
1	B	46	HIS
1	B	250	GLN
1	B	284	HIS
1	B	294	GLN
1	B	328	ASN
1	B	332	HIS
1	B	630	ASN
1	B	661	HIS
1	B	696	ASN
1	B	733	ASN
2	E	360	GLN
1	C	18	ASN
1	C	46	HIS
1	C	250	GLN
1	C	328	ASN
1	C	332	HIS
1	C	630	ASN
1	C	661	HIS
1	C	696	ASN
1	C	733	ASN
2	F	360	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 ⓘ

6 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	$\# Z > 2$
3	TTP	C	762	-	29,30,30	1.15	2 (6%)	43,47,47	1.81	8 (18%)
4	GDP	C	763	-	29,30,30	0.88	1 (3%)	45,47,47	0.83	2 (4%)
4	GDP	B	763	-	29,30,30	0.88	1 (3%)	45,47,47	0.83	2 (4%)
4	GDP	A	763	-	29,30,30	0.88	1 (3%)	45,47,47	0.83	2 (4%)
3	TTP	A	762	-	29,30,30	1.15	2 (6%)	43,47,47	1.81	8 (18%)
3	TTP	B	762	-	29,30,30	1.14	1 (3%)	43,47,47	1.81	8 (18%)

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
3	TTP	C	762	-	-	3/22/34/34	0/2/2/2
4	GDP	C	763	-	-	8/16/32/32	0/3/3/3
4	GDP	B	763	-	-	8/16/32/32	0/3/3/3
4	GDP	A	763	-	-	8/16/32/32	0/3/3/3
3	TTP	A	762	-	-	3/22/34/34	0/2/2/2
3	TTP	B	762	-	-	3/22/34/34	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	762	TTP	PG-O3G	-3.07	1.43	1.54
3	C	762	TTP	PG-O3G	-3.07	1.43	1.54
3	B	762	TTP	PG-O3G	-3.07	1.43	1.54
4	A	763	GDP	PB-O2B	-2.04	1.47	1.54
4	B	763	GDP	PB-O2B	-2.03	1.47	1.54
4	C	763	GDP	PB-O2B	-2.03	1.47	1.54
3	A	762	TTP	O4'-C4'	-2.02	1.40	1.45
3	C	762	TTP	O4'-C4'	-2.02	1.40	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	762	TTP	O4'-C1'-N1	5.48	117.59	107.86
3	B	762	TTP	O4'-C1'-N1	5.47	117.58	107.86
3	A	762	TTP	O4'-C1'-N1	5.47	117.58	107.86
3	A	762	TTP	C6-C5-C4	4.44	121.68	118.02
3	B	762	TTP	C6-C5-C4	4.43	121.67	118.02
3	C	762	TTP	C6-C5-C4	4.43	121.67	118.02
3	A	762	TTP	C5M-C5-C6	-3.56	118.03	122.85
3	C	762	TTP	C5M-C5-C6	-3.56	118.03	122.85
3	B	762	TTP	C5M-C5-C6	-3.53	118.07	122.85
3	A	762	TTP	O2A-PA-O5'	3.17	121.93	107.57
3	B	762	TTP	O2A-PA-O5'	3.17	121.92	107.57
3	C	762	TTP	O2A-PA-O5'	3.17	121.91	107.57
3	B	762	TTP	O5'-C5'-C4'	2.73	118.27	108.99
3	B	762	TTP	C2'-C1'-N1	2.72	120.63	113.81
3	A	762	TTP	C2'-C1'-N1	2.72	120.61	113.81
3	A	762	TTP	O5'-C5'-C4'	2.71	118.24	108.99
3	C	762	TTP	C2'-C1'-N1	2.71	120.59	113.81
3	C	762	TTP	O5'-C5'-C4'	2.70	118.20	108.99
3	C	762	TTP	C4-N3-C2	-2.41	124.18	127.34
3	B	762	TTP	C4-N3-C2	-2.40	124.19	127.34
3	A	762	TTP	C4-N3-C2	-2.39	124.21	127.34
4	C	763	GDP	O2B-PB-O1B	2.24	119.54	110.83
4	B	763	GDP	O2B-PB-O1B	2.23	119.54	110.83
4	A	763	GDP	O2B-PB-O1B	2.23	119.51	110.83
3	C	762	TTP	O3'-C3'-C2'	2.14	118.30	110.88
3	A	762	TTP	O3'-C3'-C2'	2.14	118.30	110.88
3	B	762	TTP	O3'-C3'-C2'	2.12	118.25	110.88
4	C	763	GDP	C2'-C3'-C4'	2.12	106.71	102.61
4	A	763	GDP	C2'-C3'-C4'	2.10	106.67	102.61
4	B	763	GDP	C2'-C3'-C4'	2.10	106.66	102.61

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	762	TTP	PB-O3B-PG-O2G
3	A	762	TTP	PB-O3B-PG-O3G
3	B	762	TTP	PB-O3B-PG-O2G
3	B	762	TTP	PB-O3B-PG-O3G
3	C	762	TTP	PB-O3B-PG-O2G
3	C	762	TTP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
4	A	763	GDP	PA-O3A-PB-O2B
4	B	763	GDP	PA-O3A-PB-O2B
4	C	763	GDP	PA-O3A-PB-O2B
4	A	763	GDP	C3'-C4'-C5'-O5'
4	B	763	GDP	C3'-C4'-C5'-O5'
4	C	763	GDP	C3'-C4'-C5'-O5'
4	A	763	GDP	O4'-C1'-N9-C4
4	B	763	GDP	O4'-C1'-N9-C4
4	C	763	GDP	O4'-C1'-N9-C4
4	A	763	GDP	O4'-C4'-C5'-O5'
4	B	763	GDP	O4'-C4'-C5'-O5'
4	C	763	GDP	O4'-C4'-C5'-O5'
4	A	763	GDP	O4'-C1'-N9-C8
4	B	763	GDP	O4'-C1'-N9-C8
4	C	763	GDP	O4'-C1'-N9-C8
4	A	763	GDP	C4'-C5'-O5'-PA
4	B	763	GDP	C4'-C5'-O5'-PA
4	C	763	GDP	C4'-C5'-O5'-PA
4	A	763	GDP	PA-O3A-PB-O1B
4	B	763	GDP	PA-O3A-PB-O1B
4	C	763	GDP	PA-O3A-PB-O1B
4	A	763	GDP	PA-O3A-PB-O3B
4	B	763	GDP	PA-O3A-PB-O3B
4	C	763	GDP	PA-O3A-PB-O3B
3	A	762	TTP	O4'-C4'-C5'-O5'
3	C	762	TTP	O4'-C4'-C5'-O5'
3	B	762	TTP	O4'-C4'-C5'-O5'

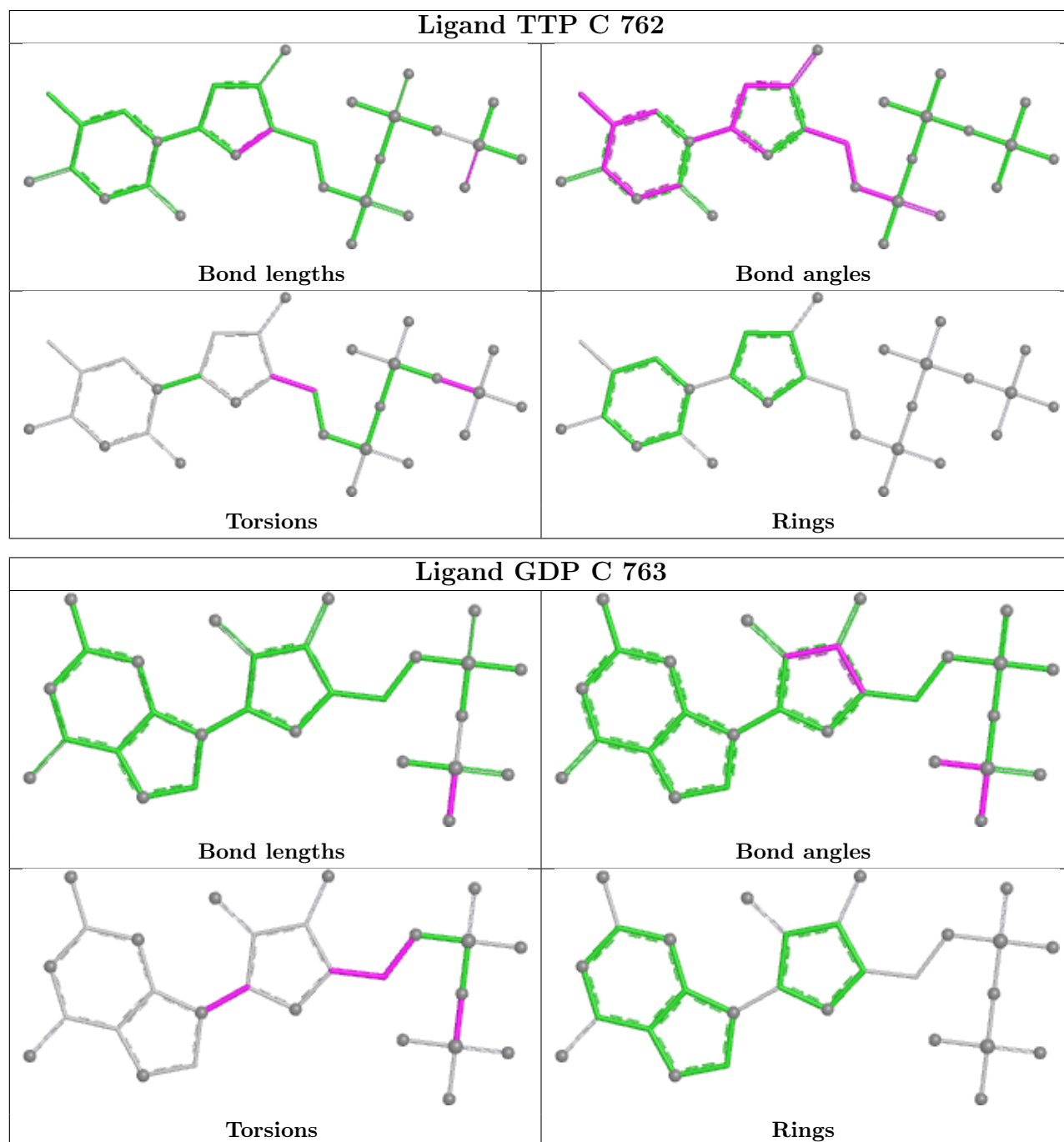
There are no ring outliers.

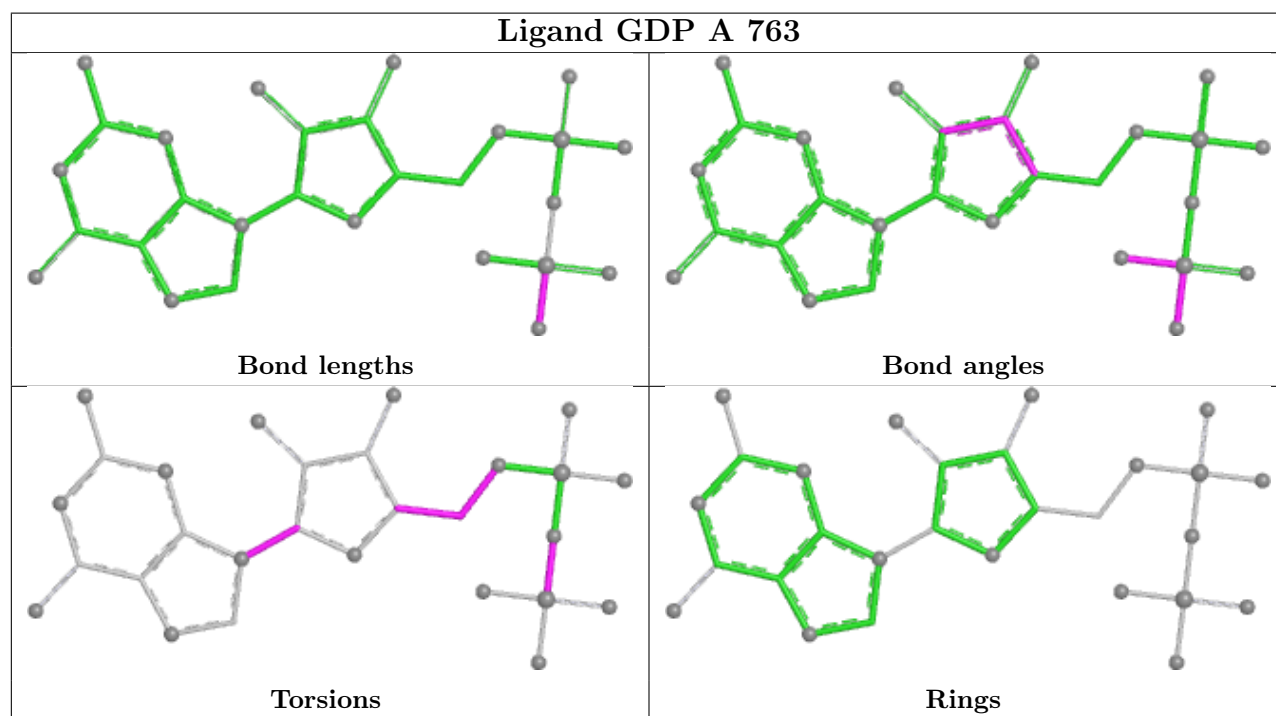
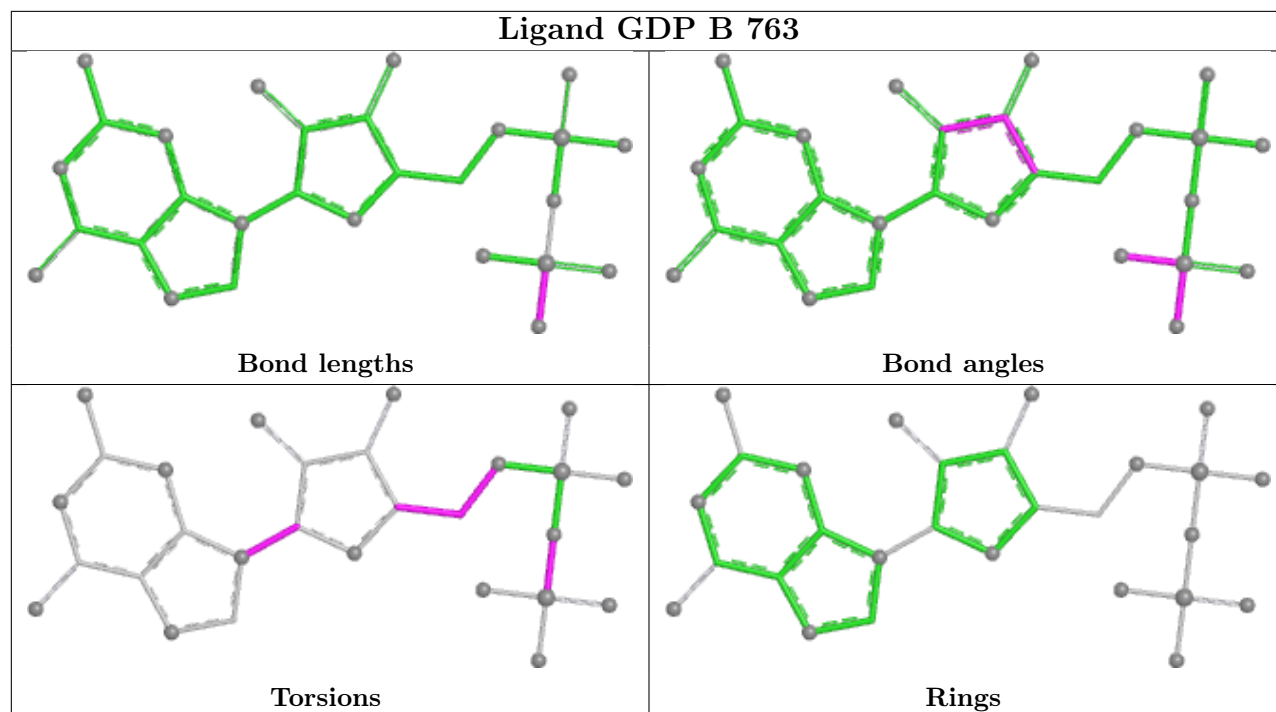
6 monomers are involved in 25 short contacts:

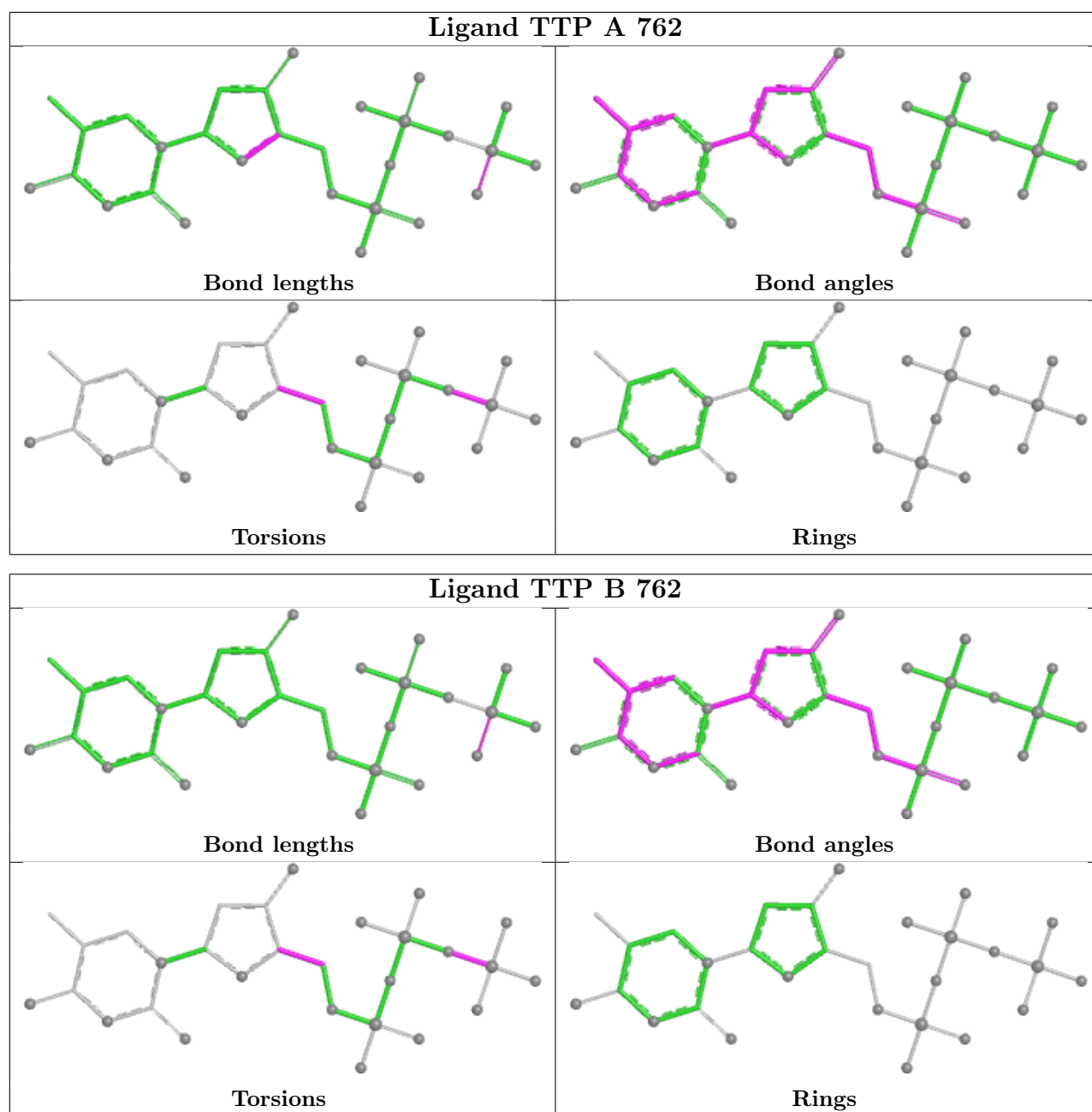
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	762	TTP	7	0
4	C	763	GDP	1	0
4	B	763	GDP	1	0
4	A	763	GDP	1	0
3	A	762	TTP	7	0
3	B	762	TTP	8	0

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.







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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	733/761 (96%)	0.40	32 (4%)	39	24	6, 21, 73, 104	0
1	B	733/761 (96%)	0.37	33 (4%)	38	24	6, 21, 73, 104	0
1	C	733/761 (96%)	0.75	81 (11%)	10	7	6, 21, 73, 104	0
2	D	16/20 (80%)	1.49	4 (25%)	2	2	43, 79, 87, 93	0
2	E	16/20 (80%)	1.31	4 (25%)	2	2	43, 79, 87, 93	0
2	F	16/20 (80%)	1.36	3 (18%)	3	2	43, 79, 87, 93	0
2	P	3/20 (15%)	2.41	2 (66%)	0	0	47, 47, 52, 56	0
All	All	2250/2363 (95%)	0.53	159 (7%)	22	14	6, 22, 79, 104	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	GLY	6.6
1	B	297	VAL	6.3
1	C	276	THR	5.7
1	B	737	GLY	5.6
1	B	296	GLY	5.4
1	C	297	VAL	5.4
1	B	273	ALA	5.3
1	C	111	GLU	5.0
1	C	324	GLY	4.8
1	C	118	HIS	4.6
1	C	273	ALA	4.5
1	C	272	GLU	4.5
1	C	13	SER	4.4
1	B	5	LEU	4.4
2	E	361	ILE	4.3
2	D	361	ILE	4.2
1	C	623	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	294	GLN	4.1
1	C	325	VAL	4.1
1	A	325	VAL	4.0
1	A	296	GLY	4.0
1	C	455	GLU	4.0
1	B	272	GLU	3.9
2	P	3	VAL	3.9
1	B	11	ASP	3.9
1	C	268	ILE	3.8
1	C	24	ARG	3.7
1	C	275	HIS	3.5
1	A	267	PRO	3.5
1	C	450	ASN	3.5
1	A	297	VAL	3.4
1	A	273	ALA	3.4
2	F	361	ILE	3.4
1	A	276	THR	3.4
1	C	11	ASP	3.4
1	C	737	GLY	3.4
1	C	267	PRO	3.4
1	C	14	THR	3.3
1	C	298	ARG	3.3
1	C	126	GLU	3.3
1	B	13	SER	3.3
1	C	301	ALA	3.3
1	C	40	GLN	3.2
1	A	737	GLY	3.2
2	E	372	ASN	3.2
1	B	274	PHE	3.2
1	B	118	HIS	3.2
1	C	326	GLU	3.2
1	C	274	PHE	3.2
1	B	450	ASN	3.1
1	B	55	THR	3.1
1	A	295	GLY	3.1
1	A	269	ARG	3.1
1	C	473	ASN	3.0
1	C	639	ARG	3.0
1	A	9	LYS	3.0
1	C	645	LYS	3.0
1	A	275	HIS	3.0
1	B	270	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	17	ILE	2.9
1	C	8	THR	2.9
1	C	392	ARG	2.9
1	C	7	VAL	2.9
1	A	5	LEU	2.8
1	C	557	GLU	2.8
1	A	274	PHE	2.8
1	A	300	GLY	2.8
2	D	367	THR	2.8
1	C	265	GLY	2.7
1	C	480	GLU	2.7
1	C	447	LYS	2.7
1	A	324	GLY	2.7
1	C	225	CYS	2.6
1	A	266	SER	2.6
1	C	5	LEU	2.6
2	P	2	LEU	2.6
2	D	360	GLN	2.6
1	B	12	GLY	2.6
1	C	120	LEU	2.6
1	C	270	GLY	2.6
1	B	276	THR	2.6
1	A	118	HIS	2.5
1	C	251	ARG	2.5
1	C	495	TYR	2.5
1	A	6	LEU	2.5
1	C	19	LEU	2.5
1	C	384	LYS	2.5
1	C	160	ARG	2.5
2	F	360	GLN	2.5
1	A	272	GLU	2.5
1	C	55	THR	2.5
1	A	291	SER	2.5
1	C	252	ALA	2.5
1	C	328	ASN	2.5
1	C	269	ARG	2.5
1	B	267	PRO	2.5
1	B	271	GLY	2.5
1	B	326	GLU	2.4
1	C	323	ARG	2.4
1	B	160	ARG	2.4
1	C	20	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	94	TYR	2.4
1	A	301	ALA	2.4
1	C	35	ASN	2.4
1	C	322	ASN	2.4
1	C	34	HIS	2.4
1	A	268	ILE	2.4
1	C	292	ALA	2.4
1	B	648	LYS	2.4
1	C	195	ARG	2.4
1	B	269	ARG	2.3
1	B	294	GLN	2.3
1	B	126	GLU	2.3
1	C	16	ARG	2.3
1	B	8	THR	2.3
1	B	187	GLU	2.3
1	A	10	ARG	2.3
1	C	253	GLY	2.3
1	C	39	SER	2.3
1	C	300	GLY	2.3
1	C	43	LEU	2.3
1	C	46	HIS	2.3
1	C	117	ASN	2.2
2	F	372	ASN	2.2
1	A	294	GLN	2.2
1	C	391	GLN	2.2
1	C	38	ILE	2.2
1	C	479	GLU	2.2
2	D	372	ASN	2.2
1	B	324	GLY	2.2
1	A	76	ASP	2.2
1	C	266	SER	2.2
1	B	480	GLU	2.2
1	C	15	GLU	2.2
1	C	271	GLY	2.2
1	B	301	ALA	2.1
1	C	327	GLY	2.1
1	C	76	ASP	2.1
1	C	407	ALA	2.1
1	A	336	GLY	2.1
1	B	225	CYS	2.1
1	B	392	ARG	2.1
1	A	271	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	509	GLY	2.1
1	C	31	GLU	2.1
1	A	13	SER	2.1
1	B	268	ILE	2.1
1	A	277	GLY	2.1
1	A	373	GLU	2.1
1	C	21	LYS	2.0
1	B	293	SER	2.0
1	C	736	ASP	2.0
2	E	370	LEU	2.0
1	C	647	SER	2.0
2	E	363	SER	2.0
1	A	630	ASN	2.0
1	C	321	ASN	2.0
1	A	11	ASP	2.0
1	C	121	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

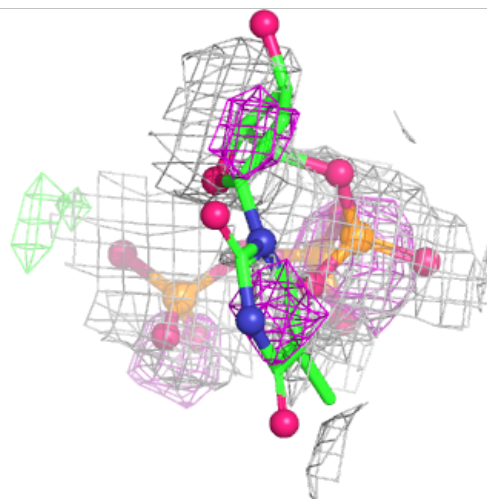
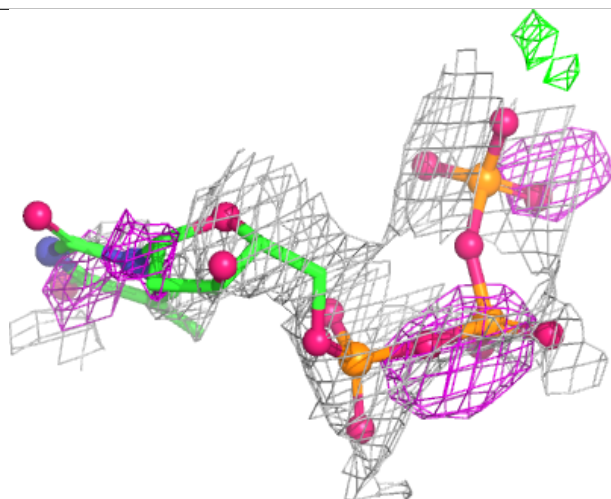
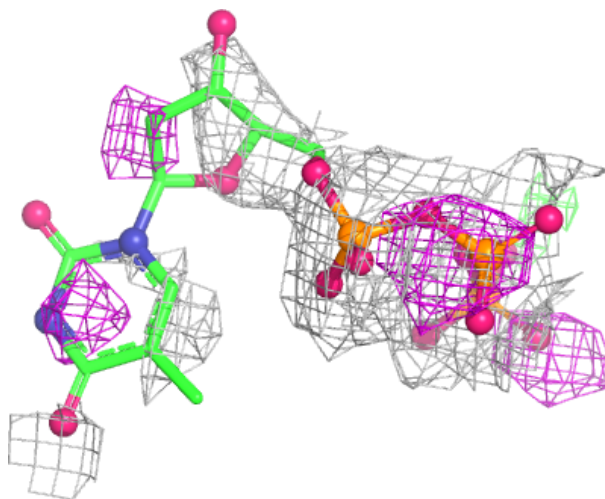
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TTP	A	762	29/29	0.61	0.20	70,71,75,75	0
3	TTP	C	762	29/29	0.61	0.20	70,71,75,75	0
3	TTP	B	762	29/29	0.63	0.18	70,71,75,75	0
4	GDP	A	763	28/28	0.65	0.45	62,62,63,63	28
4	GDP	C	763	28/28	0.67	0.52	62,62,63,63	28
4	GDP	B	763	28/28	0.73	0.43	62,62,63,63	28

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.

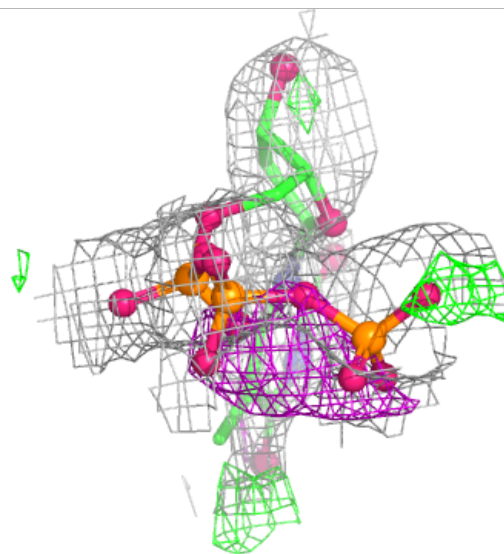
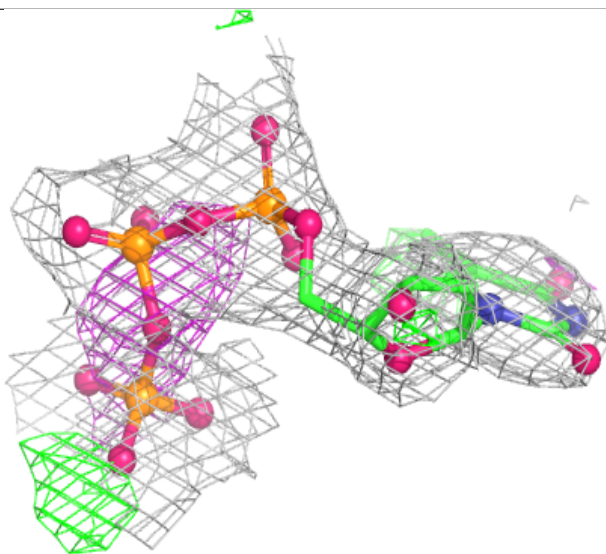
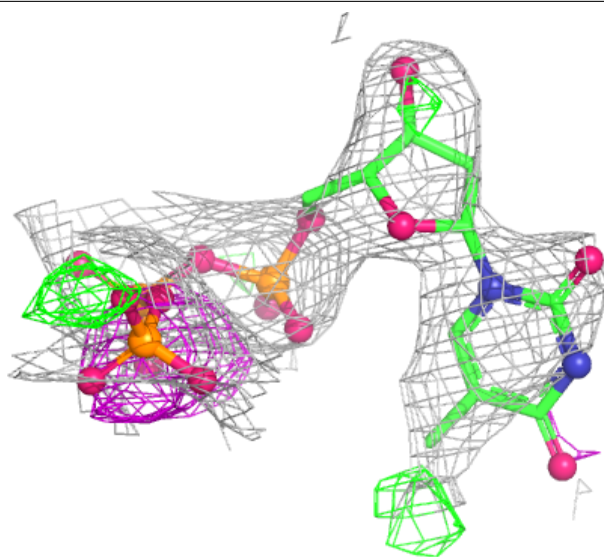
Electron density around TTP A 762:

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



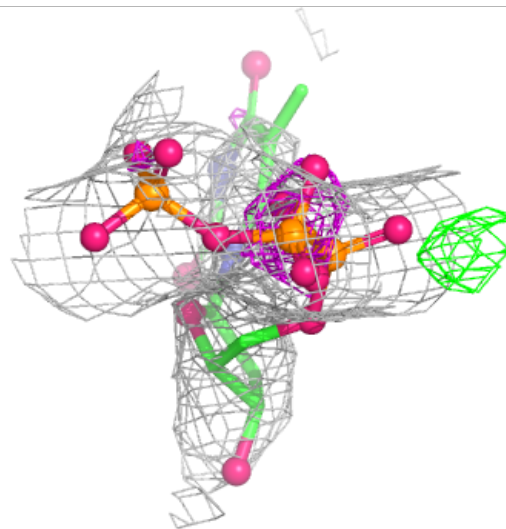
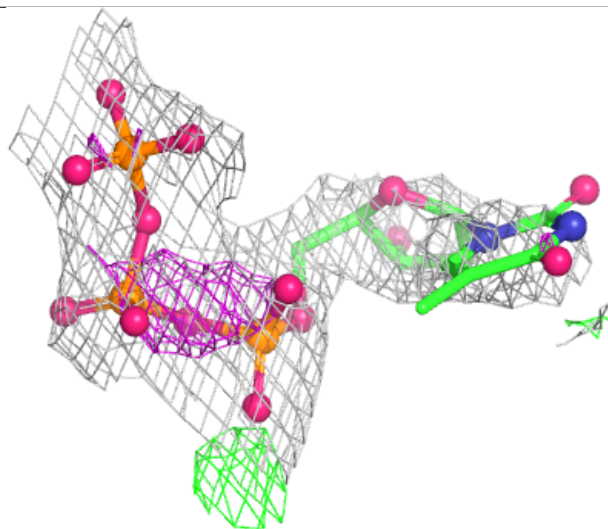
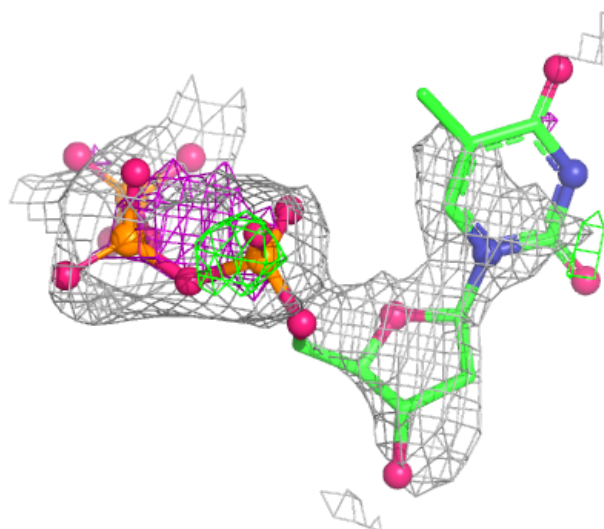
Electron density around TTP C 762:

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



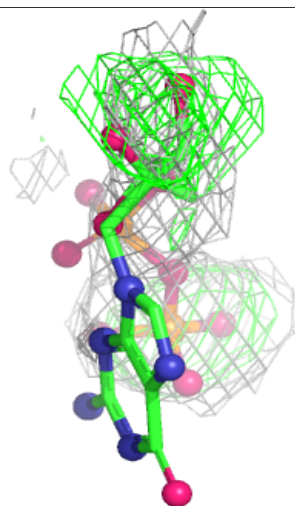
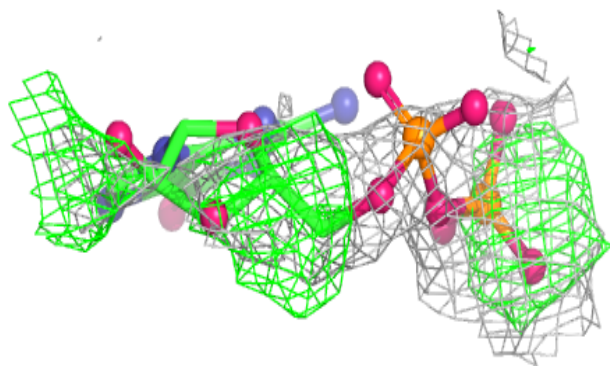
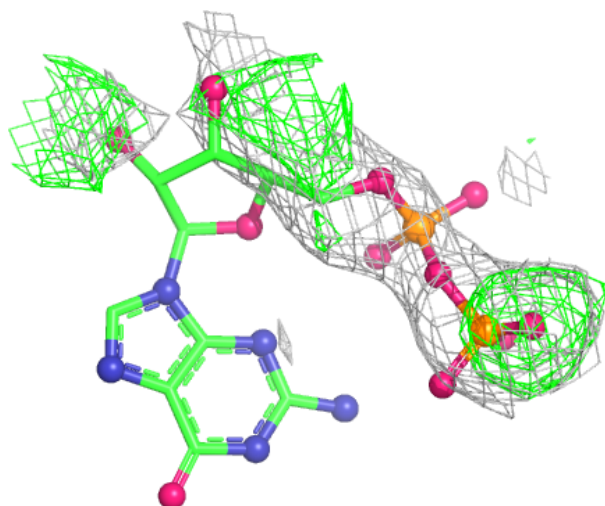
Electron density around TTP B 762:

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



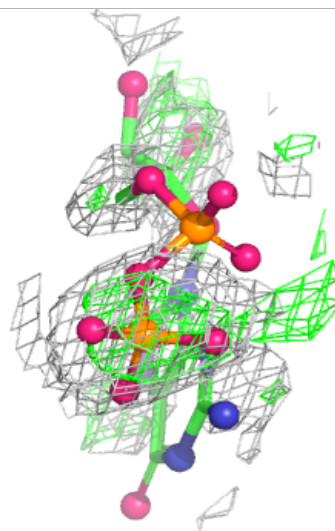
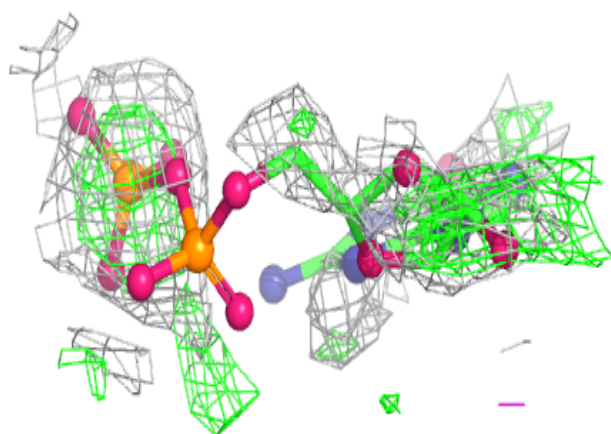
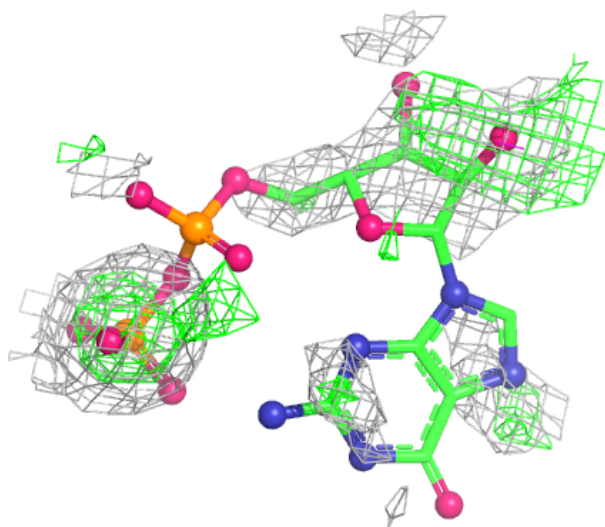
Electron density around GDP A 763:

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



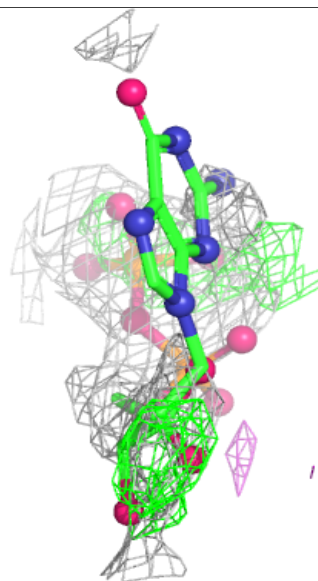
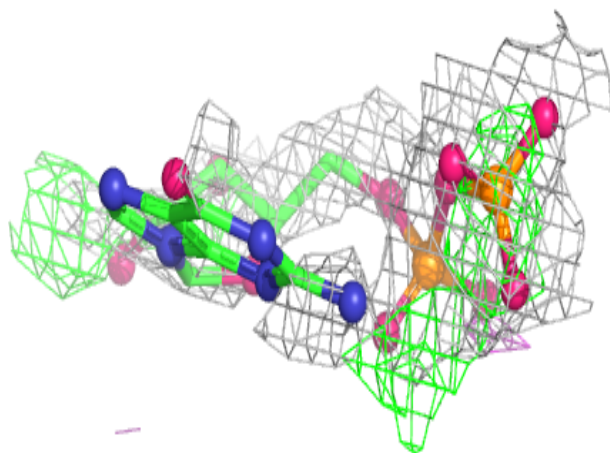
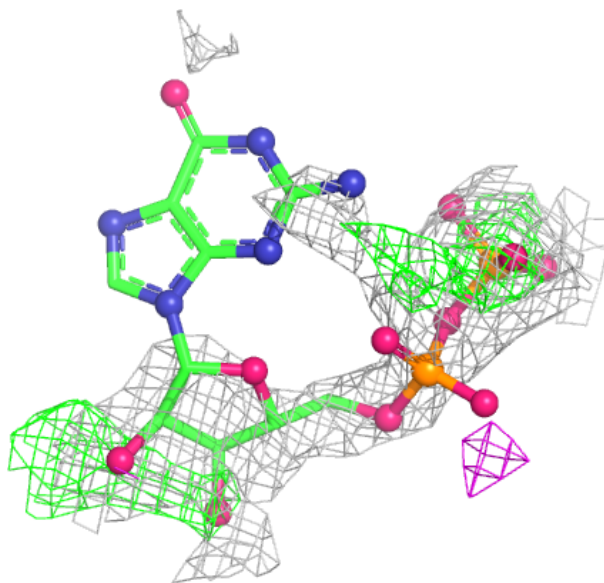
Electron density around GDP C 763:

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 763:

$2mF_o-DF_c$ (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.