



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:28 AM UTC

PDB ID : 2R1R / pdb_00002r1r
Title : RIBONUCLEOTIDE REDUCTASE R1 PROTEIN WITH DTTP OCCUPY-
ING THE SPECIFICITY SITE FROM ESCHERICHIA COLI
Authors : Eriksson, M.; Eklund, H.
Deposited on : 1997-07-21
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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

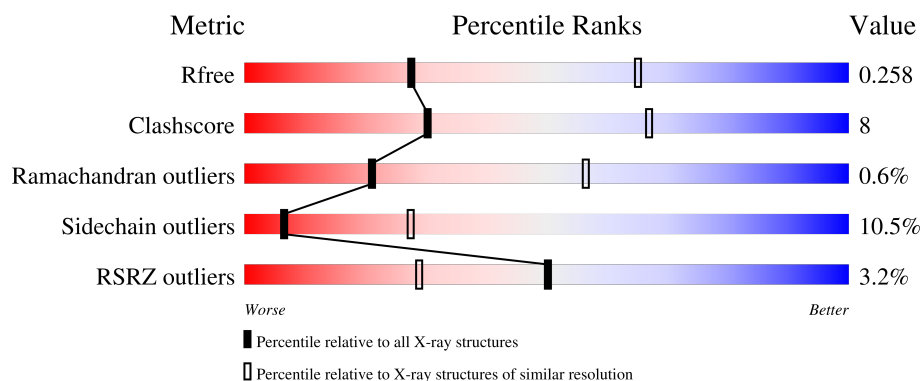
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	3% 68% 24% . .
1	B	761	2% 68% 25% . .
1	C	761	5% 68% 25% . .
2	D	20	40% 20% 5% 35%
2	E	20	40% 20% 5% 35%

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17941 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.

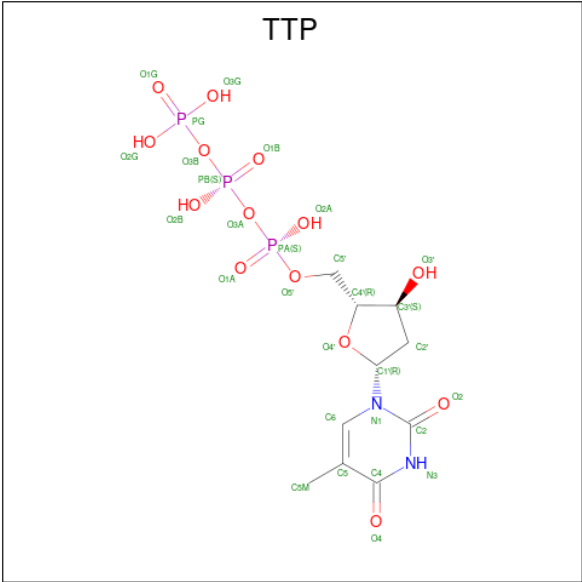
- Molecule 1 is a protein called RIBONUCLEOTIDE REDUCTASE R1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	0	0
			5837	3708	1002	1103	24			
1	B	733	Total	C	N	O	S	0	0	0
			5837	3708	1002	1103	24			
1	C	733	Total	C	N	O	S	0	0	0
			5837	3708	1002	1103	24			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	0	0	0
			104	62	15	27			
2	E	13	Total	C	N	O	0	0	0
			104	62	15	27			
2	F	13	Total	C	N	O	0	0	0
			104	62	15	27			
2	P	4	Total	C	N	O	0	0	0
			31	22	4	5			

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).

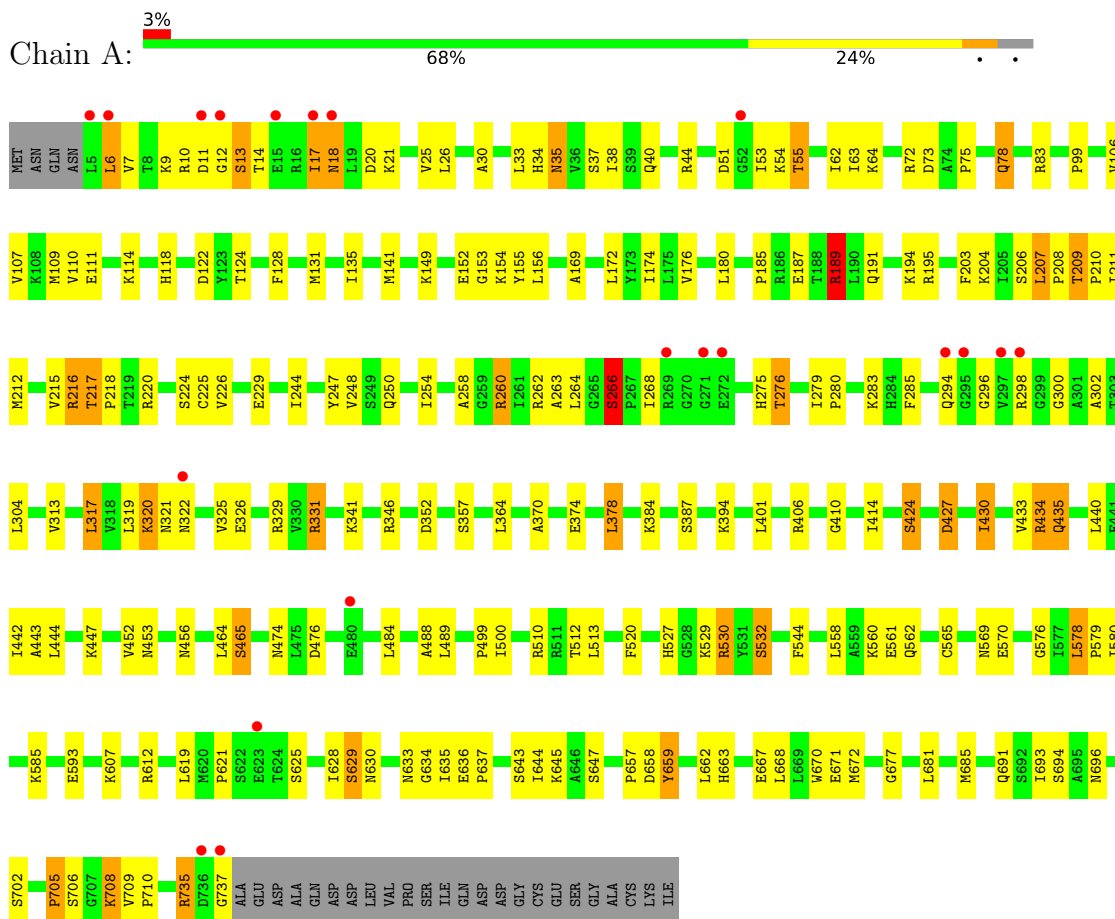


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
3	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
3	C	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

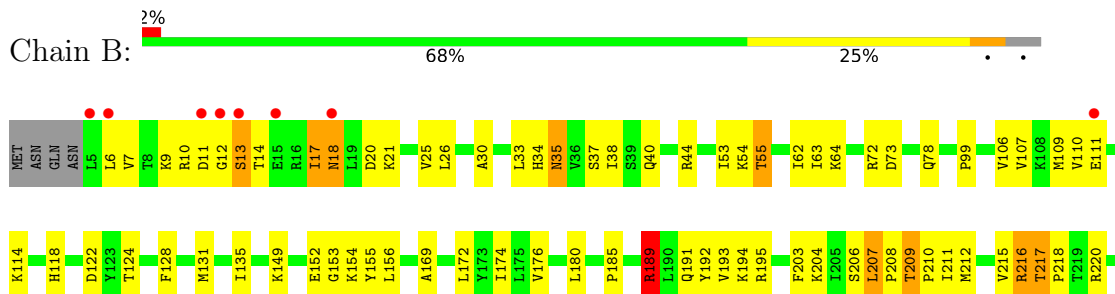
3 Residue-property plots

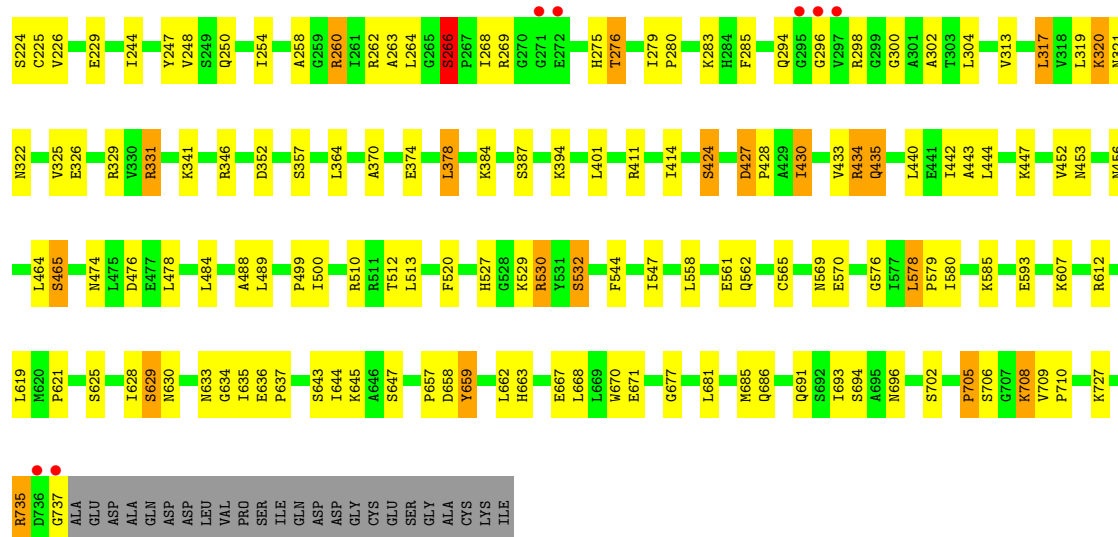
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

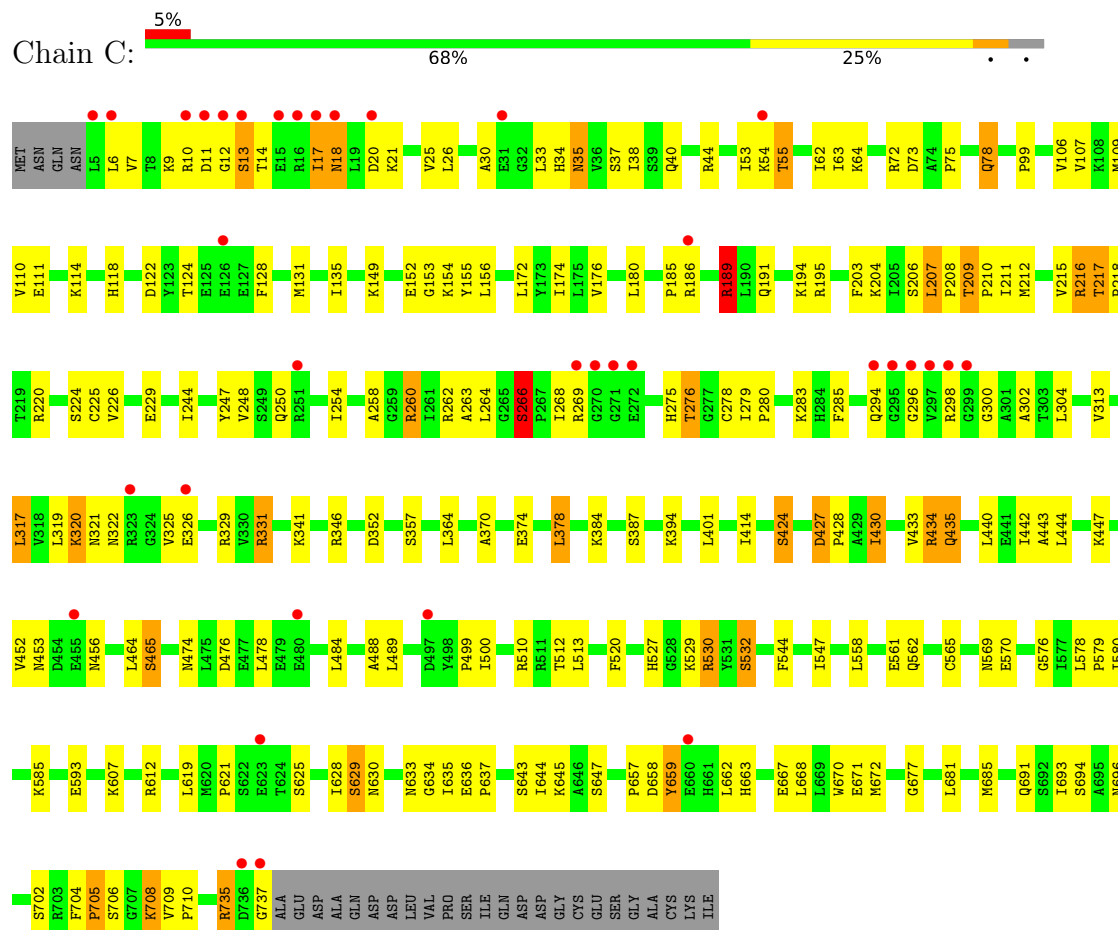


• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN



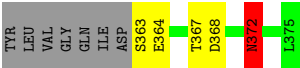


• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

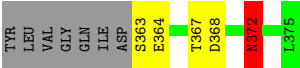


• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

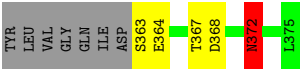




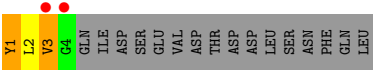
● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



● 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	227.82Å 227.82Å 343.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.02	Depositor EDS
% Data completeness (in resolution range)	83.0 (20.00-3.00) 84.7 (20.00-3.02)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.04Å)	Xtriage
Refinement program	TNT, REFMAC	Depositor
R, R_{free}	0.238 , 0.280 0.254 , 0.258	Depositor DCC
R_{free} test set	573 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	17941	wwPDB-VP
Average B, all atoms (Å ²)	5.0	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: 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	0/5965	1.30	60/8079 (0.7%)
1	B	0.41	0/5965	1.30	58/8079 (0.7%)
1	C	0.41	0/5965	1.30	58/8079 (0.7%)
2	D	0.51	0/104	1.54	1/139 (0.7%)
2	E	0.51	0/104	1.54	1/139 (0.7%)
2	F	0.52	0/104	1.54	1/139 (0.7%)
2	P	0.78	0/31	1.94	1/41 (2.4%)
All	All	0.42	0/18238	1.31	180/24695 (0.7%)

There are no bond length outliers.

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	SER	CA-C-O	10.60	132.08	120.32
1	A	13	SER	CA-C-O	10.59	132.07	120.32
1	C	13	SER	CA-C-O	10.54	132.02	120.32
1	B	464	LEU	N-CA-C	7.79	121.72	109.81
1	A	464	LEU	N-CA-C	7.78	121.71	109.81
1	C	464	LEU	N-CA-C	7.75	121.66	109.81
2	P	3	VAL	N-CA-C	7.33	124.59	109.34
1	B	544	PHE	CA-CB-CG	-7.04	106.76	113.80
1	C	544	PHE	CA-CB-CG	-7.04	106.76	113.80
1	A	544	PHE	CA-CB-CG	-7.02	106.78	113.80
1	C	331	ARG	N-CA-C	6.75	119.65	111.82
1	A	331	ARG	N-CA-C	6.75	119.64	111.82
1	B	331	ARG	N-CA-C	6.72	119.62	111.82
1	B	532	SER	N-CA-C	6.64	120.64	112.54
1	C	532	SER	N-CA-C	6.62	120.62	112.54
1	A	532	SER	N-CA-C	6.60	120.59	112.54
1	B	18	ASN	CA-CB-CG	-6.55	106.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ASN	CA-CB-CG	-6.51	106.09	112.60
1	C	18	ASN	CA-CB-CG	-6.47	106.13	112.60
1	B	209	THR	CA-C-N	6.14	125.63	119.24
1	B	209	THR	C-N-CA	6.14	125.63	119.24
1	A	209	THR	CA-C-N	6.14	125.63	119.24
1	A	209	THR	C-N-CA	6.14	125.63	119.24
1	C	209	THR	CA-C-N	6.10	125.59	119.24
1	C	209	THR	C-N-CA	6.10	125.59	119.24
1	B	185	PRO	N-CA-CB	5.91	108.50	103.35
1	B	447	LYS	CA-C-N	5.91	125.87	119.78
1	B	447	LYS	C-N-CA	5.91	125.87	119.78
1	A	185	PRO	N-CA-CB	5.89	108.48	103.35
1	B	285	PHE	CA-CB-CG	5.89	119.69	113.80
1	C	185	PRO	N-CA-CB	5.88	108.47	103.35
1	C	285	PHE	CA-CB-CG	5.87	119.67	113.80
1	A	447	LYS	CA-C-N	5.87	125.82	119.78
1	A	447	LYS	C-N-CA	5.87	125.82	119.78
1	A	285	PHE	CA-CB-CG	5.85	119.65	113.80
1	C	636	GLU	CA-C-N	5.83	123.86	119.66
1	C	636	GLU	C-N-CA	5.83	123.86	119.66
1	C	11	ASP	N-CA-CB	5.82	119.89	110.40
1	A	11	ASP	N-CA-CB	5.81	119.86	110.40
1	B	11	ASP	N-CA-CB	5.80	119.86	110.40
1	C	447	LYS	CA-C-N	5.80	125.75	119.78
1	C	447	LYS	C-N-CA	5.80	125.75	119.78
1	A	636	GLU	CA-C-N	5.79	123.83	119.66
1	A	636	GLU	C-N-CA	5.79	123.83	119.66
1	B	636	GLU	CA-C-N	5.76	123.81	119.66
1	B	636	GLU	C-N-CA	5.76	123.81	119.66
1	A	370	ALA	N-CA-C	5.71	118.71	111.69
1	B	370	ALA	N-CA-C	5.69	118.69	111.69
1	C	370	ALA	N-CA-C	5.67	118.66	111.69
1	C	217	THR	CA-C-N	5.58	125.95	119.47
1	C	217	THR	C-N-CA	5.58	125.95	119.47
1	A	424	SER	CA-C-N	5.57	125.26	119.64
1	A	424	SER	C-N-CA	5.57	125.26	119.64
1	B	298	ARG	NH1-CZ-NH2	-5.55	112.08	119.30
1	C	424	SER	CA-C-N	5.54	125.24	119.64
1	C	424	SER	C-N-CA	5.54	125.24	119.64
1	A	298	ARG	NH1-CZ-NH2	-5.54	112.09	119.30
1	C	298	ARG	NH1-CZ-NH2	-5.54	112.09	119.30
1	C	17	ILE	CB-CA-C	-5.54	103.08	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ILE	CB-CA-C	-5.54	103.08	111.33
1	B	424	SER	CA-C-N	5.54	125.23	119.64
1	B	424	SER	C-N-CA	5.54	125.23	119.64
1	A	217	THR	CA-C-N	5.53	125.88	119.47
1	A	217	THR	C-N-CA	5.53	125.88	119.47
1	B	17	ILE	CB-CA-C	-5.50	103.13	111.33
1	A	20	ASP	CA-CB-CG	-5.50	107.10	112.60
1	B	217	THR	CA-C-N	5.50	125.85	119.47
1	B	217	THR	C-N-CA	5.50	125.85	119.47
1	B	453	ASN	CA-CB-CG	-5.49	107.11	112.60
1	B	20	ASP	CA-CB-CG	-5.49	107.11	112.60
1	C	20	ASP	CA-CB-CG	-5.47	107.13	112.60
1	C	35	ASN	CA-CB-CG	-5.47	107.13	112.60
1	A	453	ASN	CA-CB-CG	-5.47	107.13	112.60
1	C	453	ASN	CA-CB-CG	-5.47	107.13	112.60
1	A	657	PRO	N-CA-CB	5.45	108.17	103.27
1	A	35	ASN	CA-CB-CG	-5.44	107.16	112.60
1	B	35	ASN	CA-CB-CG	-5.42	107.18	112.60
1	B	657	PRO	N-CA-CB	5.38	108.11	103.27
1	A	427	ASP	CA-C-N	5.37	125.19	119.28
1	A	427	ASP	C-N-CA	5.37	125.19	119.28
1	C	657	PRO	N-CA-CB	5.37	108.10	103.27
1	C	427	ASP	CA-C-N	5.37	125.19	119.28
1	C	427	ASP	C-N-CA	5.37	125.19	119.28
1	B	427	ASP	CA-C-N	5.35	125.17	119.28
1	B	427	ASP	C-N-CA	5.35	125.17	119.28
1	A	440	LEU	N-CA-C	5.34	118.81	111.54
1	C	735	ARG	N-CA-C	5.34	118.22	110.42
1	A	735	ARG	N-CA-C	5.34	118.21	110.42
1	B	440	LEU	N-CA-C	5.33	118.79	111.54
1	C	266	SER	CA-C-N	5.32	125.48	119.90
1	C	266	SER	C-N-CA	5.32	125.48	119.90
1	C	565	CYS	CA-C-N	5.32	124.77	119.24
1	C	565	CYS	C-N-CA	5.32	124.77	119.24
1	A	266	SER	CA-C-N	5.31	125.48	119.90
1	A	266	SER	C-N-CA	5.31	125.48	119.90
1	C	440	LEU	N-CA-C	5.31	118.76	111.54
1	B	735	ARG	N-CA-C	5.31	118.17	110.42
1	A	565	CYS	CA-C-N	5.29	124.75	119.24
1	A	565	CYS	C-N-CA	5.29	124.75	119.24
1	C	207	LEU	CA-C-N	5.29	125.58	119.92
1	C	207	LEU	C-N-CA	5.29	125.58	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	SER	CA-C-N	5.29	125.45	119.90
1	B	266	SER	C-N-CA	5.29	125.45	119.90
1	B	456	ASN	CA-CB-CG	-5.29	107.31	112.60
1	A	456	ASN	CA-CB-CG	-5.29	107.31	112.60
1	B	99	PRO	N-CA-CB	5.28	108.20	103.08
1	C	99	PRO	N-CA-CB	5.28	108.20	103.08
1	A	35	ASN	OD1-CG-ND2	5.27	127.87	122.60
1	B	207	LEU	CA-C-N	5.27	125.56	119.92
1	B	207	LEU	C-N-CA	5.27	125.56	119.92
1	B	500	ILE	CA-C-N	5.27	125.32	119.32
1	B	500	ILE	C-N-CA	5.27	125.32	119.32
1	A	99	PRO	N-CA-CB	5.26	108.18	103.08
1	B	35	ASN	OD1-CG-ND2	5.26	127.86	122.60
1	C	456	ASN	CA-CB-CG	-5.25	107.35	112.60
1	B	565	CYS	CA-C-N	5.25	124.70	119.24
1	B	565	CYS	C-N-CA	5.25	124.70	119.24
1	C	35	ASN	OD1-CG-ND2	5.25	127.84	122.60
1	A	207	LEU	CA-C-N	5.24	125.53	119.92
1	A	207	LEU	C-N-CA	5.24	125.53	119.92
1	A	500	ILE	CA-C-N	5.22	125.27	119.32
1	A	500	ILE	C-N-CA	5.22	125.27	119.32
1	C	705	PRO	N-CA-CB	5.21	107.81	103.17
1	C	500	ILE	CA-C-N	5.20	125.25	119.32
1	C	500	ILE	C-N-CA	5.20	125.25	119.32
1	A	298	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	B	298	ARG	NE-CZ-NH1	5.18	126.69	121.50
1	C	298	ARG	NE-CZ-NH1	5.18	126.68	121.50
2	E	372	ASN	CA-CB-CG	-5.15	107.45	112.60
1	A	705	PRO	N-CA-CB	5.15	107.75	103.17
1	B	593	GLU	CA-C-N	5.15	125.36	120.31
1	B	593	GLU	C-N-CA	5.15	125.36	120.31
1	B	710	PRO	N-CA-CB	5.14	108.12	103.34
2	D	372	ASN	CA-CB-CG	-5.13	107.47	112.60
2	F	372	ASN	CA-CB-CG	-5.13	107.47	112.60
1	A	593	GLU	CA-C-N	5.12	125.33	120.31
1	A	593	GLU	C-N-CA	5.12	125.33	120.31
1	B	705	PRO	N-CA-CB	5.12	107.73	103.17
1	C	153	GLY	N-CA-C	5.11	118.68	112.49
1	C	637	PRO	N-CA-CB	5.11	105.88	103.22
1	A	710	PRO	N-CA-CB	5.11	108.09	103.34
1	B	153	GLY	N-CA-C	5.10	118.66	112.49
1	C	710	PRO	N-CA-CB	5.10	108.09	103.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	737	GLY	N-CA-C	-5.10	98.52	113.30
1	C	672	MET	CA-C-N	5.10	124.59	119.19
1	C	672	MET	C-N-CA	5.10	124.59	119.19
1	C	737	GLY	N-CA-C	-5.09	98.53	113.30
1	C	659	TYR	CA-C-N	5.09	127.82	120.38
1	C	659	TYR	C-N-CA	5.09	127.82	120.38
1	A	737	GLY	N-CA-C	-5.09	98.54	113.30
1	C	593	GLU	CA-C-N	5.09	125.30	120.31
1	C	593	GLU	C-N-CA	5.09	125.30	120.31
1	A	637	PRO	N-CA-CB	5.08	105.86	103.22
1	A	153	GLY	N-CA-C	5.07	118.63	112.49
1	A	12	GLY	CA-C-N	-5.07	114.94	122.74
1	A	12	GLY	C-N-CA	-5.07	114.94	122.74
1	A	659	TYR	CA-C-N	5.06	127.77	120.38
1	A	659	TYR	C-N-CA	5.06	127.77	120.38
1	B	659	TYR	CA-C-N	5.06	127.77	120.38
1	B	659	TYR	C-N-CA	5.06	127.77	120.38
1	B	12	GLY	CA-C-N	-5.05	114.96	122.74
1	B	12	GLY	C-N-CA	-5.05	114.96	122.74
1	B	357	SER	CA-C-N	5.05	124.50	119.24
1	B	357	SER	C-N-CA	5.05	124.50	119.24
1	B	637	PRO	N-CA-CB	5.05	105.85	103.22
1	B	203	PHE	N-CA-C	5.05	118.56	111.90
1	A	357	SER	CA-C-N	5.04	124.49	119.24
1	A	357	SER	C-N-CA	5.04	124.49	119.24
1	A	672	MET	CA-C-N	5.04	124.54	119.19
1	A	672	MET	C-N-CA	5.04	124.54	119.19
1	C	203	PHE	N-CA-C	5.04	118.55	111.90
1	C	357	SER	CA-C-N	5.04	124.48	119.24
1	C	357	SER	C-N-CA	5.04	124.48	119.24
1	C	12	GLY	CA-C-N	-5.04	114.98	122.74
1	C	12	GLY	C-N-CA	-5.04	114.98	122.74
1	A	203	PHE	N-CA-C	5.03	118.54	111.90
1	A	578	LEU	CA-C-N	5.01	125.03	119.32
1	A	578	LEU	C-N-CA	5.01	125.03	119.32
1	B	578	LEU	CA-C-N	5.00	125.02	119.32
1	B	578	LEU	C-N-CA	5.00	125.02	119.32

There are no chirality outliers.

There are no planarity outliers.

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	5837	0	5762	96	0
1	B	5837	0	5762	101	0
1	C	5837	0	5762	98	0
2	D	104	0	88	2	0
2	E	104	0	88	2	0
2	F	104	0	88	2	0
2	P	31	0	34	1	0
3	A	29	0	13	3	0
3	B	29	0	13	2	0
3	C	29	0	13	2	0
All	All	17941	0	17623	300	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 8.

All (300) 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:558:LEU:HD23	1:B:612:ARG:HG2	1.56	0.85
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.56	0.85
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.56	0.84
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.60	0.84
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.60	0.83
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.59	0.82
1:C:7:VAL:HG23	1:C:17:ILE:HG12	1.63	0.81
1:B:7:VAL:HG23	1:B:17:ILE:HG12	1.63	0.81
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.65	0.79
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.65	0.79
1:A:7:VAL:HG23	1:A:17:ILE:HG12	1.63	0.78
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.65	0.77
1:C:128:PHE:HA	1:C:131:MET:HE3	1.69	0.75
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.69	0.74
1:B:128:PHE:HA	1:B:131:MET:HE3	1.69	0.74
1:A:561:GLU:HG2	1:A:562:GLN:HG3	1.70	0.74
1:C:561:GLU:HG2	1:C:562:GLN:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:SER:HB2	1:C:489:LEU:HD11	1.69	0.73
1:A:128:PHE:HA	1:A:131:MET:HE3	1.69	0.73
1:B:465:SER:HB2	1:B:489:LEU:HD11	1.69	0.73
1:B:561:GLU:HG2	1:B:562:GLN:HG3	1.70	0.71
1:A:268:ILE:HD11	1:A:275:HIS:HA	1.74	0.69
1:A:322:ASN:HA	1:A:331:ARG:HE	1.57	0.69
1:B:322:ASN:HA	1:B:331:ARG:HE	1.57	0.69
1:C:322:ASN:HA	1:C:331:ARG:HE	1.57	0.69
1:B:208:PRO:HG2	1:B:211:ILE:HD12	1.76	0.68
1:C:208:PRO:HG2	1:C:211:ILE:HD12	1.76	0.68
1:B:268:ILE:HD11	1:B:275:HIS:HA	1.74	0.68
1:C:268:ILE:HD11	1:C:275:HIS:HA	1.74	0.67
1:A:215:VAL:O	1:A:216:ARG:HB3	1.94	0.67
1:A:208:PRO:HG2	1:A:211:ILE:HD12	1.76	0.67
1:C:215:VAL:O	1:C:216:ARG:HB3	1.94	0.67
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.77	0.66
2:E:372:ASN:H	2:E:372:ASN:ND2	1.93	0.66
1:A:578:LEU:HB3	1:A:579:PRO:HD2	1.77	0.65
1:B:215:VAL:O	1:B:216:ARG:HB3	1.94	0.65
2:D:372:ASN:H	2:D:372:ASN:ND2	1.93	0.64
1:B:578:LEU:HB3	1:B:579:PRO:HD2	1.77	0.64
2:F:372:ASN:ND2	2:F:372:ASN:H	1.93	0.64
1:A:217:THR:HB	1:A:218:PRO:HD2	1.81	0.62
1:C:317:LEU:HD23	1:C:401:LEU:HD23	1.83	0.61
1:B:317:LEU:HD23	1:B:401:LEU:HD23	1.82	0.61
1:C:217:THR:HB	1:C:218:PRO:HD2	1.81	0.61
1:B:209:THR:N	1:B:210:PRO:HD2	2.16	0.61
1:B:217:THR:HB	1:B:218:PRO:HD2	1.81	0.61
1:B:18:ASN:HB2	1:B:21:LYS:HE3	1.83	0.61
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.83	0.61
1:A:18:ASN:HB2	1:A:21:LYS:HE3	1.83	0.61
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.83	0.60
1:C:209:THR:N	1:C:210:PRO:HD2	2.16	0.60
1:A:317:LEU:HD23	1:A:401:LEU:HD23	1.82	0.60
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.83	0.60
1:A:209:THR:N	1:A:210:PRO:HD2	2.16	0.60
1:C:18:ASN:HB2	1:C:21:LYS:HE3	1.83	0.60
1:A:26:LEU:HB3	1:A:38:ILE:HD12	1.84	0.59
1:B:427:ASP:HB3	1:B:430:ILE:HD12	1.84	0.59
1:C:260:ARG:HH22	1:C:434:ARG:NH2	2.01	0.59
1:A:109:MET:HE3	1:A:114:LYS:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ASP:HB3	1:A:430:ILE:HD12	1.84	0.59
1:B:26:LEU:HB3	1:B:38:ILE:HD12	1.84	0.59
1:C:26:LEU:HB3	1:C:38:ILE:HD12	1.84	0.58
1:C:427:ASP:HB3	1:C:430:ILE:HD12	1.84	0.58
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.85	0.58
1:A:576:GLY:HA3	1:A:607:LYS:HE2	1.86	0.58
1:A:260:ARG:HH22	1:A:434:ARG:NH2	2.01	0.58
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.85	0.58
1:C:109:MET:HE3	1:C:114:LYS:HB2	1.85	0.58
1:B:109:MET:HE3	1:B:114:LYS:HB2	1.85	0.58
1:B:260:ARG:HH22	1:B:434:ARG:NH2	2.01	0.58
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.85	0.57
1:C:576:GLY:HA3	1:C:607:LYS:HE2	1.86	0.57
1:A:260:ARG:HH22	1:A:434:ARG:HH21	1.53	0.57
1:B:576:GLY:HA3	1:B:607:LYS:HE2	1.86	0.57
1:B:275:HIS:CE1	3:B:762:TTP:H1'	2.40	0.57
1:C:275:HIS:CE1	3:C:762:TTP:H1'	2.40	0.57
1:A:530:ARG:HH11	1:A:667:GLU:HB2	1.70	0.56
1:B:585:LYS:H	1:B:585:LYS:HD3	1.69	0.56
1:C:530:ARG:HH11	1:C:667:GLU:HB2	1.70	0.56
1:A:275:HIS:CE1	3:A:762:TTP:H1'	2.40	0.56
1:B:530:ARG:HH11	1:B:667:GLU:HB2	1.70	0.56
1:A:7:VAL:CG2	1:A:17:ILE:HG12	2.35	0.56
1:A:585:LYS:H	1:A:585:LYS:HD3	1.69	0.56
1:B:34:HIS:O	1:B:35:ASN:HB2	2.05	0.56
1:C:260:ARG:HH22	1:C:434:ARG:HH21	1.53	0.56
1:C:585:LYS:H	1:C:585:LYS:HD3	1.69	0.56
1:A:34:HIS:O	1:A:35:ASN:HB2	2.05	0.55
1:C:34:HIS:O	1:C:35:ASN:HB2	2.05	0.55
1:B:276:THR:HG23	1:B:280:PRO:HG2	1.87	0.55
1:A:276:THR:HG23	1:A:280:PRO:HG2	1.87	0.55
1:B:260:ARG:HH22	1:B:434:ARG:HH21	1.53	0.55
1:A:180:LEU:HD13	1:A:488:ALA:HB1	1.89	0.55
1:C:276:THR:HG23	1:C:280:PRO:HG2	1.88	0.55
1:B:180:LEU:HD13	1:B:488:ALA:HB1	1.89	0.54
1:C:180:LEU:HD13	1:C:488:ALA:HB1	1.89	0.54
1:B:7:VAL:CG2	1:B:17:ILE:HG12	2.35	0.53
1:C:7:VAL:CG2	1:C:17:ILE:HG12	2.35	0.53
1:A:263:ALA:O	1:A:266:SER:HB2	2.09	0.53
1:B:263:ALA:O	1:B:266:SER:HB2	2.09	0.53
1:C:152:GLU:HA	1:C:156:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ALA:O	1:C:266:SER:HB2	2.09	0.52
1:B:152:GLU:HA	1:B:156:LEU:HD12	1.92	0.52
1:C:37:SER:HB3	1:C:40:GLN:HG2	1.92	0.51
1:C:37:SER:OG	1:C:40:GLN:HG2	2.10	0.51
1:A:37:SER:HB3	1:A:40:GLN:HG2	1.93	0.51
1:B:37:SER:OG	1:B:40:GLN:HG2	2.10	0.51
1:A:152:GLU:HA	1:A:156:LEU:HD12	1.92	0.51
1:A:37:SER:OG	1:A:40:GLN:HG2	2.10	0.51
1:A:172:LEU:O	1:A:176:VAL:HG23	2.11	0.51
1:A:215:VAL:O	1:A:216:ARG:CB	2.59	0.51
1:B:37:SER:HB3	1:B:40:GLN:HG2	1.93	0.51
1:C:215:VAL:O	1:C:216:ARG:CB	2.59	0.51
1:C:172:LEU:O	1:C:176:VAL:HG23	2.11	0.51
1:A:244:ILE:O	1:A:248:VAL:HG22	2.11	0.51
1:B:37:SER:CB	1:B:40:GLN:HG2	2.41	0.51
1:B:172:LEU:O	1:B:176:VAL:HG23	2.11	0.51
1:C:37:SER:CB	1:C:40:GLN:HG2	2.41	0.51
1:A:260:ARG:NH2	1:A:434:ARG:HH21	2.09	0.50
1:A:279:ILE:HB	1:A:280:PRO:CD	2.37	0.50
1:A:37:SER:CB	1:A:40:GLN:HG2	2.41	0.50
1:B:215:VAL:O	1:B:216:ARG:CB	2.59	0.50
1:A:633:ASN:O	1:A:634:GLY:C	2.55	0.50
1:B:633:ASN:O	1:B:634:GLY:C	2.55	0.50
1:C:260:ARG:NH2	1:C:434:ARG:HH21	2.09	0.50
1:C:244:ILE:O	1:C:248:VAL:HG22	2.11	0.50
1:C:250:GLN:HE22	1:C:499:PRO:HG3	1.77	0.50
1:B:244:ILE:O	1:B:248:VAL:HG22	2.11	0.49
1:B:250:GLN:HE22	1:B:499:PRO:HG3	1.77	0.49
1:C:633:ASN:O	1:C:634:GLY:C	2.55	0.49
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.94	0.49
1:B:260:ARG:NH2	1:B:434:ARG:HH21	2.09	0.49
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.95	0.49
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.94	0.48
1:B:527:HIS:O	1:B:529:LYS:HE2	2.14	0.48
1:A:527:HIS:O	1:A:529:LYS:HE2	2.14	0.48
1:C:670:TRP:CH2	1:C:735:ARG:HB2	2.49	0.48
1:A:250:GLN:HE22	1:A:499:PRO:HG3	1.77	0.48
1:B:670:TRP:CH2	1:B:735:ARG:HB2	2.48	0.48
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.94	0.48
1:C:527:HIS:O	1:C:529:LYS:HE2	2.14	0.48
1:A:670:TRP:CH2	1:A:735:ARG:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HB2	1:A:212:MET:HE3	1.94	0.48
1:B:155:TYR:HE1	1:B:209:THR:HG23	1.78	0.48
1:B:207:LEU:HB2	1:B:212:MET:HE3	1.95	0.48
1:C:520:PHE:HB3	1:C:635:ILE:HA	1.95	0.48
1:C:207:LEU:HB2	1:C:212:MET:HE3	1.95	0.48
1:A:18:ASN:CB	1:A:21:LYS:HE3	2.44	0.48
1:A:279:ILE:HD12	1:A:319:LEU:HD21	1.96	0.47
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.95	0.47
1:B:670:TRP:CZ2	1:B:735:ARG:HB2	2.49	0.47
1:C:155:TYR:CE1	1:C:209:THR:HG23	2.50	0.47
1:A:155:TYR:CE1	1:A:209:THR:HG23	2.50	0.47
1:A:229:GLU:OE2	1:A:260:ARG:NH1	2.48	0.47
1:A:346:ARG:HD2	1:A:352:ASP:O	2.15	0.47
1:A:560:LYS:HA	2:P:1:TYR:N	2.29	0.47
1:A:670:TRP:CZ2	1:A:735:ARG:HB2	2.49	0.47
1:C:670:TRP:CZ2	1:C:735:ARG:HB2	2.50	0.47
1:A:155:TYR:HE1	1:A:209:THR:HG23	1.78	0.47
1:B:18:ASN:CB	1:B:21:LYS:HE3	2.44	0.46
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.96	0.46
1:A:705:PRO:O	1:A:706:SER:HB2	2.15	0.46
1:B:705:PRO:O	1:B:706:SER:HB2	2.15	0.46
1:C:30:ALA:HA	1:C:33:LEU:HD12	1.96	0.46
1:C:279:ILE:HB	1:C:280:PRO:CD	2.37	0.46
1:C:705:PRO:O	1:C:706:SER:HB2	2.15	0.46
1:C:30:ALA:HB2	1:C:38:ILE:HD11	1.97	0.46
1:C:155:TYR:HE1	1:C:209:THR:HG23	1.79	0.46
1:C:474:ASN:OD1	1:C:476:ASP:HB2	2.15	0.46
1:A:254:ILE:O	1:A:302:ALA:HA	2.16	0.46
1:A:474:ASN:OD1	1:A:476:ASP:HB2	2.15	0.46
1:B:279:ILE:HD12	1:B:319:LEU:HD21	1.96	0.46
1:C:18:ASN:CB	1:C:21:LYS:HE3	2.44	0.46
1:B:30:ALA:HB2	1:B:38:ILE:HD11	1.97	0.46
1:B:346:ARG:HD2	1:B:352:ASP:O	2.15	0.46
1:C:229:GLU:OE2	1:C:260:ARG:NH1	2.48	0.46
1:A:434:ARG:O	1:A:435:GLN:HB3	2.16	0.46
1:B:254:ILE:O	1:B:302:ALA:HA	2.16	0.46
1:B:279:ILE:HB	1:B:280:PRO:CD	2.37	0.46
1:C:279:ILE:HD12	1:C:319:LEU:HD21	1.96	0.46
1:A:21:LYS:O	1:A:25:VAL:HG23	2.16	0.46
1:B:229:GLU:OE2	1:B:260:ARG:NH1	2.48	0.46
1:C:434:ARG:O	1:C:435:GLN:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ALA:HA	1:A:33:LEU:HD12	1.96	0.46
1:B:155:TYR:CE1	1:B:209:THR:HG23	2.50	0.46
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.97	0.46
1:A:30:ALA:HB2	1:A:38:ILE:HD11	1.97	0.46
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.97	0.46
1:B:658:ASP:HB3	1:B:662:LEU:HD12	1.97	0.46
1:C:21:LYS:O	1:C:25:VAL:HG23	2.16	0.46
1:A:658:ASP:HB3	1:A:662:LEU:HD12	1.97	0.45
1:B:442:ILE:HA	1:B:691:GLN:OE1	2.16	0.45
1:C:658:ASP:HB3	1:C:662:LEU:HD12	1.98	0.45
1:A:442:ILE:HA	1:A:691:GLN:OE1	2.16	0.45
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.97	0.45
1:B:474:ASN:OD1	1:B:476:ASP:HB2	2.15	0.45
1:C:254:ILE:O	1:C:302:ALA:HA	2.16	0.45
1:B:434:ARG:O	1:B:435:GLN:HB3	2.16	0.45
1:A:275:HIS:ND1	3:A:762:TTP:H1'	2.31	0.45
1:C:346:ARG:HD2	1:C:352:ASP:O	2.15	0.45
1:B:329:ARG:HG3	1:B:331:ARG:NH2	2.32	0.45
1:B:489:LEU:HB3	1:B:513:LEU:HD22	1.98	0.45
1:C:442:ILE:HA	1:C:691:GLN:OE1	2.16	0.45
1:C:275:HIS:ND1	3:C:762:TTP:H1'	2.31	0.45
1:C:489:LEU:HB3	1:C:513:LEU:HD22	1.98	0.45
1:A:489:LEU:HB3	1:A:513:LEU:HD22	1.98	0.45
1:B:21:LYS:O	1:B:25:VAL:HG23	2.16	0.45
1:B:191:GLN:O	1:B:195:ARG:HG3	2.17	0.45
1:C:191:GLN:O	1:C:195:ARG:HG3	2.17	0.45
1:A:191:GLN:O	1:A:195:ARG:HG3	2.16	0.44
1:A:659:TYR:CE1	1:A:663:HIS:HB3	2.52	0.44
1:A:172:LEU:C	1:A:172:LEU:HD23	2.43	0.44
1:B:275:HIS:ND1	3:B:762:TTP:H1'	2.31	0.44
1:C:659:TYR:CE1	1:C:663:HIS:HB3	2.52	0.44
1:A:9:LYS:HA	1:A:55:THR:OG1	2.17	0.44
1:B:9:LYS:HA	1:B:55:THR:OG1	2.17	0.44
1:B:172:LEU:C	1:B:172:LEU:HD23	2.43	0.44
1:C:329:ARG:HG3	1:C:331:ARG:NH2	2.32	0.44
1:A:329:ARG:HG3	1:A:331:ARG:NH2	2.32	0.44
1:A:187:GLU:OE2	1:C:186:ARG:HD2	2.18	0.44
1:A:681:LEU:O	1:A:685:MET:HG3	2.18	0.44
1:B:668:LEU:HB2	1:B:671:GLU:HG3	2.00	0.44
1:C:374:GLU:HG3	1:C:378:LEU:HD11	2.00	0.44
1:C:668:LEU:HB2	1:C:671:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:681:LEU:O	1:C:685:MET:HG3	2.18	0.44
1:B:659:TYR:CE1	1:B:663:HIS:HB3	2.52	0.43
1:C:9:LYS:HA	1:C:55:THR:OG1	2.17	0.43
1:A:374:GLU:HG3	1:A:378:LEU:HD11	2.00	0.43
1:A:532:SER:HA	1:A:677:GLY:HA3	2.00	0.43
1:B:558:LEU:HD23	1:B:612:ARG:CG	2.38	0.43
1:A:320:LYS:O	1:A:321:ASN:C	2.62	0.43
1:A:668:LEU:HB2	1:A:671:GLU:HG3	2.00	0.43
1:C:172:LEU:HD23	1:C:172:LEU:C	2.43	0.43
1:A:558:LEU:HD23	1:A:612:ARG:CG	2.38	0.43
1:B:681:LEU:O	1:B:685:MET:HG3	2.18	0.43
1:C:621:PRO:HD3	1:C:694:SER:OG	2.19	0.43
2:F:368:ASP:O	2:F:372:ASN:ND2	2.51	0.43
1:A:621:PRO:HD3	1:A:694:SER:OG	2.19	0.43
1:B:374:GLU:HG3	1:B:378:LEU:HD11	2.00	0.43
1:C:558:LEU:HD23	1:C:612:ARG:CG	2.38	0.43
1:A:708:LYS:HB3	1:A:708:LYS:HE3	1.90	0.42
1:B:106:VAL:O	1:B:110:VAL:HG23	2.19	0.42
1:C:106:VAL:O	1:C:110:VAL:HG23	2.19	0.42
1:B:122:ASP:O	1:B:189:ARG:NH2	2.52	0.42
1:B:532:SER:HA	1:B:677:GLY:HA3	2.00	0.42
1:B:621:PRO:HD3	1:B:694:SER:OG	2.19	0.42
1:C:122:ASP:O	1:C:189:ARG:NH2	2.52	0.42
1:C:320:LYS:O	1:C:321:ASN:C	2.62	0.42
1:B:578:LEU:HB3	1:B:579:PRO:CD	2.48	0.42
2:E:368:ASP:O	2:E:372:ASN:ND2	2.51	0.42
1:A:106:VAL:O	1:A:110:VAL:HG23	2.19	0.42
1:A:122:ASP:O	1:A:189:ARG:NH2	2.53	0.42
1:B:226:VAL:HG21	1:B:247:TYR:CD1	2.55	0.42
1:C:569:ASN:H	1:C:569:ASN:ND2	2.18	0.42
1:C:578:LEU:HB3	1:C:579:PRO:CD	2.48	0.42
1:C:532:SER:HA	1:C:677:GLY:HA3	2.01	0.42
1:C:708:LYS:HB3	1:C:708:LYS:HE3	1.90	0.42
1:A:226:VAL:HG21	1:A:247:TYR:CD1	2.55	0.42
1:C:427:ASP:HA	1:C:428:PRO:HD2	1.93	0.42
2:D:368:ASP:O	2:D:372:ASN:ND2	2.51	0.42
1:B:569:ASN:H	1:B:569:ASN:ND2	2.18	0.41
1:C:269:ARG:HG3	1:C:269:ARG:O	2.20	0.41
1:A:313:VAL:HG22	1:A:317:LEU:HD22	2.02	0.41
1:B:169:ALA:O	1:B:172:LEU:HB3	2.21	0.41
1:B:320:LYS:O	1:B:321:ASN:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:VAL:HG21	1:C:247:TYR:CD1	2.55	0.41
1:A:275:HIS:HD1	3:A:762:TTP:H1'	1.86	0.41
1:B:260:ARG:NH2	1:B:434:ARG:NH2	2.68	0.41
1:B:427:ASP:HA	1:B:428:PRO:HD2	1.93	0.41
1:A:107:VAL:O	1:A:111:GLU:HG3	2.20	0.41
1:C:313:VAL:HG22	1:C:317:LEU:HD22	2.02	0.41
1:A:62:ILE:HG13	1:A:63:ILE:N	2.36	0.41
1:A:629:SER:O	1:A:630:ASN:C	2.64	0.41
1:B:62:ILE:HG13	1:B:63:ILE:N	2.36	0.41
1:B:269:ARG:O	1:B:269:ARG:HG3	2.21	0.41
1:A:169:ALA:O	1:A:172:LEU:HB3	2.21	0.41
1:B:411:ARG:HH11	1:B:411:ARG:HD3	1.68	0.41
1:C:62:ILE:HG13	1:C:63:ILE:N	2.36	0.41
1:A:569:ASN:ND2	1:A:569:ASN:H	2.18	0.41
1:B:217:THR:HB	1:B:218:PRO:CD	2.50	0.41
1:C:7:VAL:HG23	1:C:17:ILE:CG1	2.43	0.41
1:C:278:CYS:O	1:C:279:ILE:C	2.64	0.41
1:A:6:LEU:HB2	1:A:51:ASP:CG	2.46	0.41
1:B:107:VAL:O	1:B:111:GLU:HG3	2.21	0.41
1:B:192:TYR:O	1:B:193:VAL:C	2.64	0.41
1:C:75:PRO:O	1:C:78:GLN:HB2	2.21	0.41
1:C:260:ARG:NH2	1:C:434:ARG:NH2	2.68	0.41
1:B:708:LYS:HB3	1:B:708:LYS:HE3	1.90	0.40
1:A:75:PRO:O	1:A:78:GLN:HB2	2.21	0.40
1:B:313:VAL:HG22	1:B:317:LEU:HD22	2.02	0.40
1:B:320:LYS:HE3	1:B:411:ARG:HB2	2.03	0.40
1:C:478:LEU:HD13	1:C:547:ILE:HG13	2.04	0.40
1:C:704:PHE:HA	1:C:705:PRO:HD3	1.94	0.40
1:A:406:ARG:O	1:A:410:GLY:N	2.48	0.40
1:B:321:ASN:O	1:B:329:ARG:NE	2.46	0.40
1:B:478:LEU:HD13	1:B:547:ILE:HG13	2.04	0.40
1:B:629:SER:O	1:B:630:ASN:C	2.64	0.40
1:B:686:GLN:CD	1:B:727:LYS:HD2	2.47	0.40
1:C:107:VAL:O	1:C:111:GLU:HG3	2.21	0.40
1:A:83:ARG:HG2	1:A:141:MET:HG3	2.03	0.40
1:B:7:VAL:HG23	1:B:17:ILE:CG1	2.43	0.40
1:C:629:SER:O	1:C:630:ASN:C	2.64	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%)	669 (92%)	58 (8%)	4 (0%)	24	60
1	B	731/761 (96%)	669 (92%)	58 (8%)	4 (0%)	24	60
1	C	731/761 (96%)	669 (92%)	58 (8%)	4 (0%)	24	60
2	D	11/20 (55%)	10 (91%)	1 (9%)	0	100	100
2	E	11/20 (55%)	10 (91%)	1 (9%)	0	100	100
2	F	11/20 (55%)	10 (91%)	1 (9%)	0	100	100
2	P	2/20 (10%)	0	1 (50%)	1 (50%)	0	0
All	All	2228/2363 (94%)	2037 (91%)	178 (8%)	13 (1%)	21	56

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	B	216	ARG
1	C	216	ARG
1	A	296	GLY
1	B	296	GLY
1	C	296	GLY
1	A	189	ARG
1	B	189	ARG
1	C	189	ARG
1	A	300	GLY
1	B	300	GLY
1	C	300	GLY
2	P	3	VAL

5.3.2 Protein sidechains

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	628/651 (96%)	565 (90%)	63 (10%)	7	29
1	B	628/651 (96%)	565 (90%)	63 (10%)	7	29
1	C	628/651 (96%)	565 (90%)	63 (10%)	7	29
2	D	13/19 (68%)	9 (69%)	4 (31%)	0	1
2	E	13/19 (68%)	9 (69%)	4 (31%)	0	1
2	F	13/19 (68%)	9 (69%)	4 (31%)	0	1
2	P	3/19 (16%)	1 (33%)	2 (67%)	0	0
All	All	1926/2029 (95%)	1723 (90%)	203 (10%)	6	27

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	10	ARG
1	A	13	SER
1	A	14	THR
1	A	44	ARG
1	A	53	ILE
1	A	54	LYS
1	A	55	THR
1	A	64	LYS
1	A	72	ARG
1	A	73	ASP
1	A	78	GLN
1	A	118	HIS
1	A	124	THR
1	A	149	LYS
1	A	154	LYS
1	A	189	ARG
1	A	194	LYS
1	A	204	LYS
1	A	206	SER
1	A	220	ARG
1	A	224	SER
1	A	225	CYS
1	A	260	ARG

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Mol	Chain	Res	Type
1	A	262	ARG
1	A	264	LEU
1	A	266	SER
1	A	276	THR
1	A	283	LYS
1	A	294	GLN
1	A	317	LEU
1	A	320	LYS
1	A	325	VAL
1	A	326	GLU
1	A	341	LYS
1	A	364	LEU
1	A	378	LEU
1	A	384	LYS
1	A	387	SER
1	A	394	LYS
1	A	414	ILE
1	A	424	SER
1	A	430	ILE
1	A	434	ARG
1	A	435	GLN
1	A	452	VAL
1	A	465	SER
1	A	484	LEU
1	A	510	ARG
1	A	530	ARG
1	A	570	GLU
1	A	580	ILE
1	A	625	SER
1	A	628	ILE
1	A	629	SER
1	A	643	SER
1	A	644	ILE
1	A	645	LYS
1	A	647	SER
1	A	696	ASN
1	A	702	SER
1	A	708	LYS
1	A	709	VAL
2	D	363	SER
2	D	364	GLU
2	D	367	THR

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Mol	Chain	Res	Type
2	D	372	ASN
1	B	6	LEU
1	B	10	ARG
1	B	13	SER
1	B	14	THR
1	B	44	ARG
1	B	53	ILE
1	B	54	LYS
1	B	55	THR
1	B	64	LYS
1	B	72	ARG
1	B	73	ASP
1	B	78	GLN
1	B	118	HIS
1	B	124	THR
1	B	149	LYS
1	B	154	LYS
1	B	189	ARG
1	B	194	LYS
1	B	204	LYS
1	B	206	SER
1	B	220	ARG
1	B	224	SER
1	B	225	CYS
1	B	260	ARG
1	B	262	ARG
1	B	264	LEU
1	B	266	SER
1	B	276	THR
1	B	283	LYS
1	B	294	GLN
1	B	317	LEU
1	B	320	LYS
1	B	325	VAL
1	B	326	GLU
1	B	341	LYS
1	B	364	LEU
1	B	378	LEU
1	B	384	LYS
1	B	387	SER
1	B	394	LYS
1	B	414	ILE

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Mol	Chain	Res	Type
1	B	424	SER
1	B	430	ILE
1	B	434	ARG
1	B	435	GLN
1	B	452	VAL
1	B	465	SER
1	B	484	LEU
1	B	510	ARG
1	B	530	ARG
1	B	570	GLU
1	B	580	ILE
1	B	625	SER
1	B	628	ILE
1	B	629	SER
1	B	643	SER
1	B	644	ILE
1	B	645	LYS
1	B	647	SER
1	B	696	ASN
1	B	702	SER
1	B	708	LYS
1	B	709	VAL
2	E	363	SER
2	E	364	GLU
2	E	367	THR
2	E	372	ASN
1	C	6	LEU
1	C	10	ARG
1	C	13	SER
1	C	14	THR
1	C	44	ARG
1	C	53	ILE
1	C	54	LYS
1	C	55	THR
1	C	64	LYS
1	C	72	ARG
1	C	73	ASP
1	C	78	GLN
1	C	118	HIS
1	C	124	THR
1	C	149	LYS
1	C	154	LYS

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Mol	Chain	Res	Type
1	C	189	ARG
1	C	194	LYS
1	C	204	LYS
1	C	206	SER
1	C	220	ARG
1	C	224	SER
1	C	225	CYS
1	C	260	ARG
1	C	262	ARG
1	C	264	LEU
1	C	266	SER
1	C	276	THR
1	C	283	LYS
1	C	294	GLN
1	C	317	LEU
1	C	320	LYS
1	C	325	VAL
1	C	326	GLU
1	C	341	LYS
1	C	364	LEU
1	C	378	LEU
1	C	384	LYS
1	C	387	SER
1	C	394	LYS
1	C	414	ILE
1	C	424	SER
1	C	430	ILE
1	C	434	ARG
1	C	435	GLN
1	C	452	VAL
1	C	465	SER
1	C	484	LEU
1	C	510	ARG
1	C	530	ARG
1	C	570	GLU
1	C	580	ILE
1	C	625	SER
1	C	628	ILE
1	C	629	SER
1	C	643	SER
1	C	644	ILE
1	C	645	LYS

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Mol	Chain	Res	Type
1	C	647	SER
1	C	696	ASN
1	C	702	SER
1	C	708	LYS
1	C	709	VAL
2	F	363	SER
2	F	364	GLU
2	F	367	THR
2	F	372	ASN
2	P	1	TYR
2	P	2	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	130	GLN
1	A	170	GLN
1	A	250	GLN
1	A	275	HIS
1	A	328	ASN
1	A	416	ASN
1	A	569	ASN
1	A	627	GLN
1	A	732	GLN
2	D	372	ASN
1	B	130	GLN
1	B	170	GLN
1	B	250	GLN
1	B	275	HIS
1	B	284	HIS
1	B	328	ASN
1	B	569	ASN
1	B	627	GLN
1	B	732	GLN
2	E	372	ASN
1	C	130	GLN
1	C	250	GLN
1	C	328	ASN
1	C	569	ASN
1	C	627	GLN
1	C	732	GLN

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Mol	Chain	Res	Type
2	F	372	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 ⓘ

3 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	B	762	-	29,30,30	1.84	4 (13%)	43,47,47	1.30	5 (11%)
3	TTP	A	762	-	29,30,30	1.86	4 (13%)	43,47,47	1.31	5 (11%)
3	TTP	C	762	-	29,30,30	1.87	4 (13%)	43,47,47	1.30	5 (11%)

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	B	762	-	-	1/22/34/34	0/2/2/2
3	TTP	A	762	-	-	1/22/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTP	C	762	-	-	1/22/34/34	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	762	TTP	PB-O3B	7.87	1.68	1.59
3	A	762	TTP	PB-O3B	7.80	1.67	1.59
3	B	762	TTP	PB-O3B	7.74	1.67	1.59
3	B	762	TTP	PG-O1G	2.69	1.58	1.50
3	C	762	TTP	PB-O3A	2.68	1.62	1.59
3	A	762	TTP	PG-O1G	2.66	1.58	1.50
3	C	762	TTP	PG-O1G	2.64	1.58	1.50
3	A	762	TTP	PB-O3A	2.61	1.62	1.59
3	B	762	TTP	PB-O3A	2.58	1.62	1.59
3	A	762	TTP	PA-O2A	-2.16	1.45	1.55
3	C	762	TTP	PA-O2A	-2.14	1.45	1.55
3	B	762	TTP	PA-O2A	-2.14	1.45	1.55

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	762	TTP	C6-C5-C4	4.17	121.46	118.02
3	C	762	TTP	C6-C5-C4	4.11	121.41	118.02
3	B	762	TTP	C6-C5-C4	4.10	121.40	118.02
3	A	762	TTP	C5M-C5-C6	-3.61	117.96	122.85
3	B	762	TTP	C5M-C5-C6	-3.61	117.97	122.85
3	C	762	TTP	C5M-C5-C6	-3.59	117.98	122.85
3	B	762	TTP	O3'-C3'-C4'	-2.40	100.96	110.07
3	A	762	TTP	O3'-C3'-C4'	-2.40	100.96	110.07
3	C	762	TTP	O3'-C3'-C4'	-2.40	100.98	110.07
3	A	762	TTP	O3A-PB-O1B	-2.24	103.97	110.70
3	C	762	TTP	O3A-PB-O1B	-2.22	104.02	110.70
3	B	762	TTP	O3A-PB-O1B	-2.22	104.04	110.70
3	C	762	TTP	C4-N3-C2	-2.05	124.65	127.34
3	A	762	TTP	C4-N3-C2	-2.04	124.66	127.34
3	B	762	TTP	C4-N3-C2	-2.03	124.68	127.34

There are no chirality outliers.

All (3) torsion outliers are listed below:

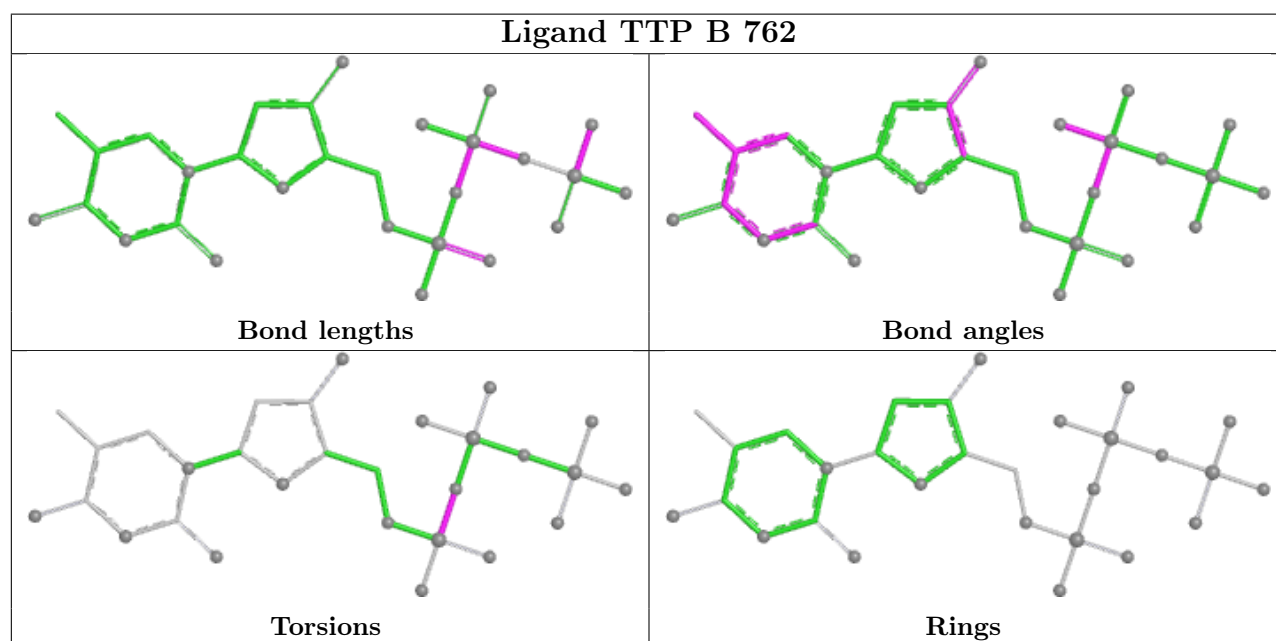
Mol	Chain	Res	Type	Atoms
3	A	762	TTP	PB-O3A-PA-O1A
3	B	762	TTP	PB-O3A-PA-O1A
3	C	762	TTP	PB-O3A-PA-O1A

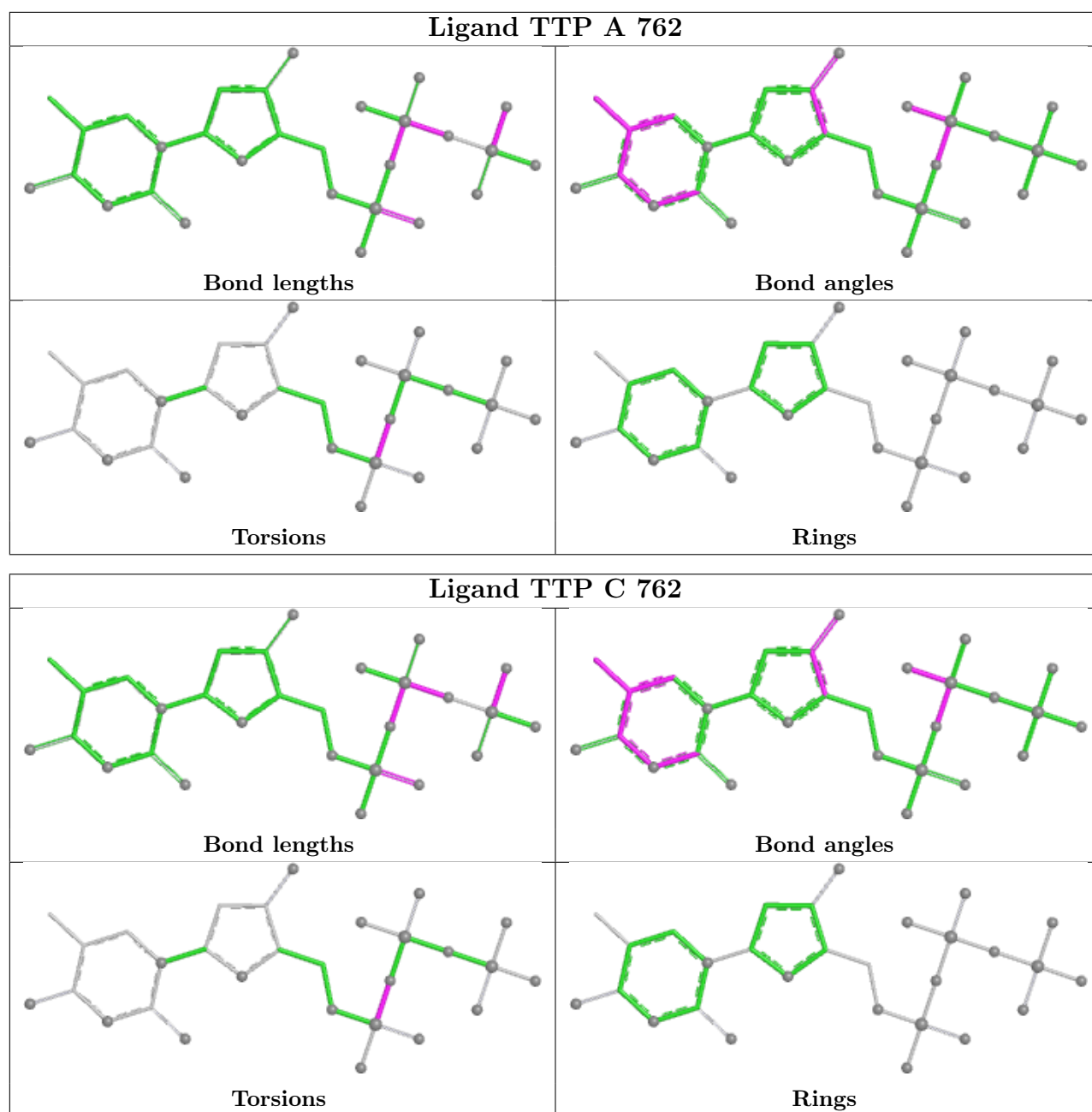
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	762	TTP	2	0
3	A	762	TTP	3	0
3	C	762	TTP	2	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%)	-0.21	20 (2%) 56 33	2, 6, 7, 9	0
1	B	733/761 (96%)	-0.15	15 (2%) 65 41	2, 6, 7, 9	0
1	C	733/761 (96%)	0.04	35 (4%) 35 19	2, 6, 7, 9	0
2	D	13/20 (65%)	0.31	0 100 100	4, 6, 7, 7	0
2	E	13/20 (65%)	0.15	0 100 100	4, 6, 7, 7	0
2	F	13/20 (65%)	0.09	0 100 100	4, 6, 7, 7	0
2	P	4/20 (20%)	1.05	2 (50%) 0 0	2, 2, 2, 3	0
All	All	2242/2363 (94%)	-0.10	72 (3%) 50 29	2, 6, 7, 9	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	737	GLY	5.5
1	B	11	ASP	5.0
1	A	11	ASP	4.5
1	C	271	GLY	4.4
1	B	737	GLY	4.3
1	A	6	LEU	4.3
1	B	295	GLY	4.1
1	C	272	GLU	4.1
1	C	18	ASN	4.0
1	C	11	ASP	4.0
1	C	10	ARG	4.0
1	A	18	ASN	3.9
1	A	12	GLY	3.8
1	B	18	ASN	3.8
1	C	16	ARG	3.7
1	C	298	ARG	3.7
1	C	13	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	271	GLY	3.6
1	B	12	GLY	3.4
1	B	296	GLY	3.4
1	A	737	GLY	3.3
1	C	20	ASP	3.2
1	C	270	GLY	3.1
1	C	269	ARG	3.1
1	A	272	GLU	3.1
1	C	736	ASP	3.0
1	B	272	GLU	2.9
1	C	5	LEU	2.9
1	B	13	SER	2.8
1	B	297	VAL	2.8
1	C	31	GLU	2.8
1	B	5	LEU	2.8
1	A	295	GLY	2.7
1	A	736	ASP	2.7
1	C	497	ASP	2.7
1	B	111	GLU	2.7
1	C	295	GLY	2.7
1	A	298	ARG	2.7
1	A	294	GLN	2.7
1	C	186	ARG	2.7
1	C	17	ILE	2.6
1	A	271	GLY	2.5
1	C	297	VAL	2.5
1	C	623	GLU	2.5
1	B	6	LEU	2.5
1	C	12	GLY	2.5
1	B	15	GLU	2.4
1	C	294	GLN	2.4
1	A	5	LEU	2.4
1	C	6	LEU	2.4
1	C	296	GLY	2.4
1	C	480	GLU	2.3
1	A	322	ASN	2.3
1	C	323	ARG	2.3
1	A	17	ILE	2.3
1	A	15	GLU	2.2
1	C	326	GLU	2.2
1	C	251	ARG	2.2
1	C	54	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	P	4	GLY	2.1
1	A	52	GLY	2.1
1	A	623	GLU	2.1
1	C	15	GLU	2.1
1	C	126	GLU	2.1
1	A	480	GLU	2.1
2	P	3	VAL	2.1
1	A	269	ARG	2.1
1	C	660	GLU	2.1
1	B	736	ASP	2.1
1	C	455	GLU	2.1
1	A	297	VAL	2.0
1	C	299	GLY	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](#)

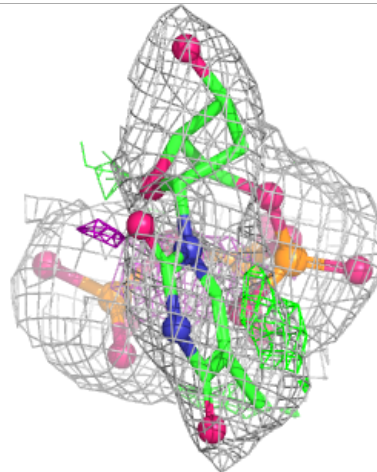
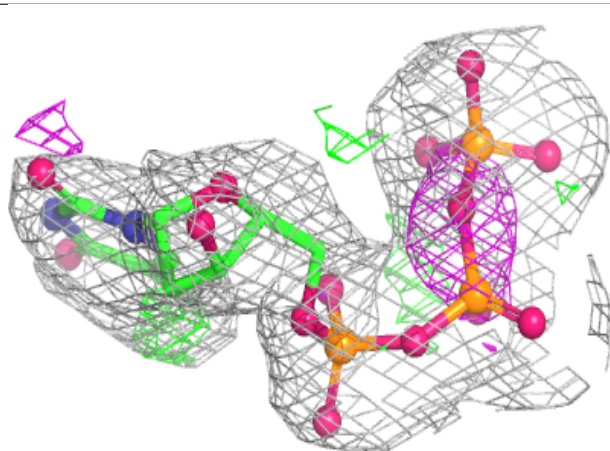
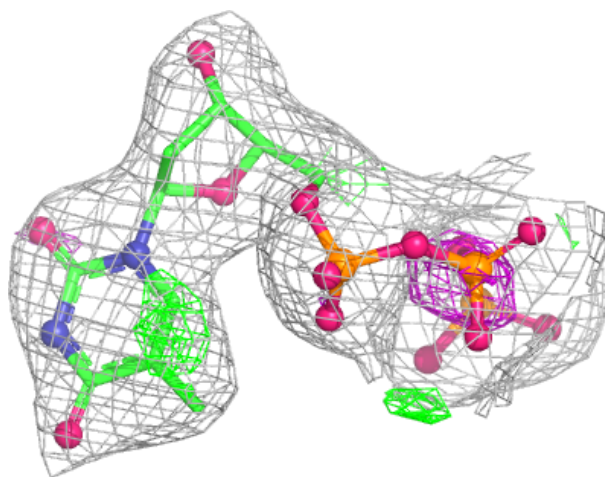
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	762	29/29	0.91	0.11	2,2,5,6	0
3	TTP	B	762	29/29	0.92	0.11	2,2,5,6	0
3	TTP	A	762	29/29	0.94	0.10	2,2,5,6	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.

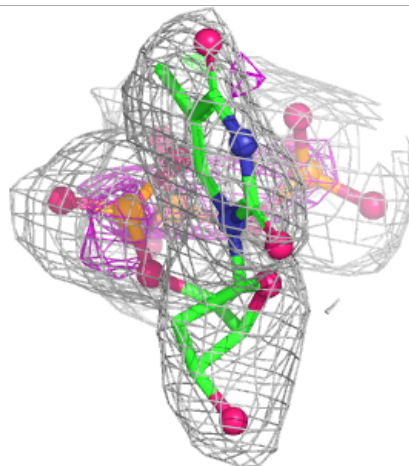
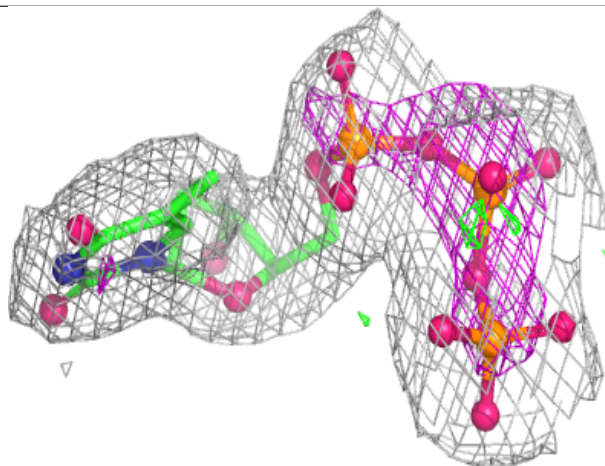
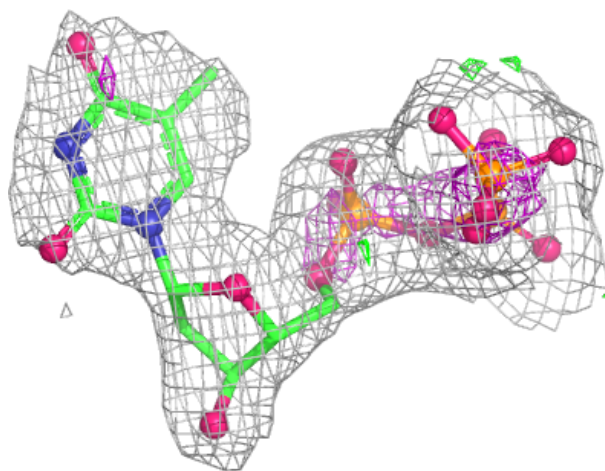
Electron density around TTP C 762:

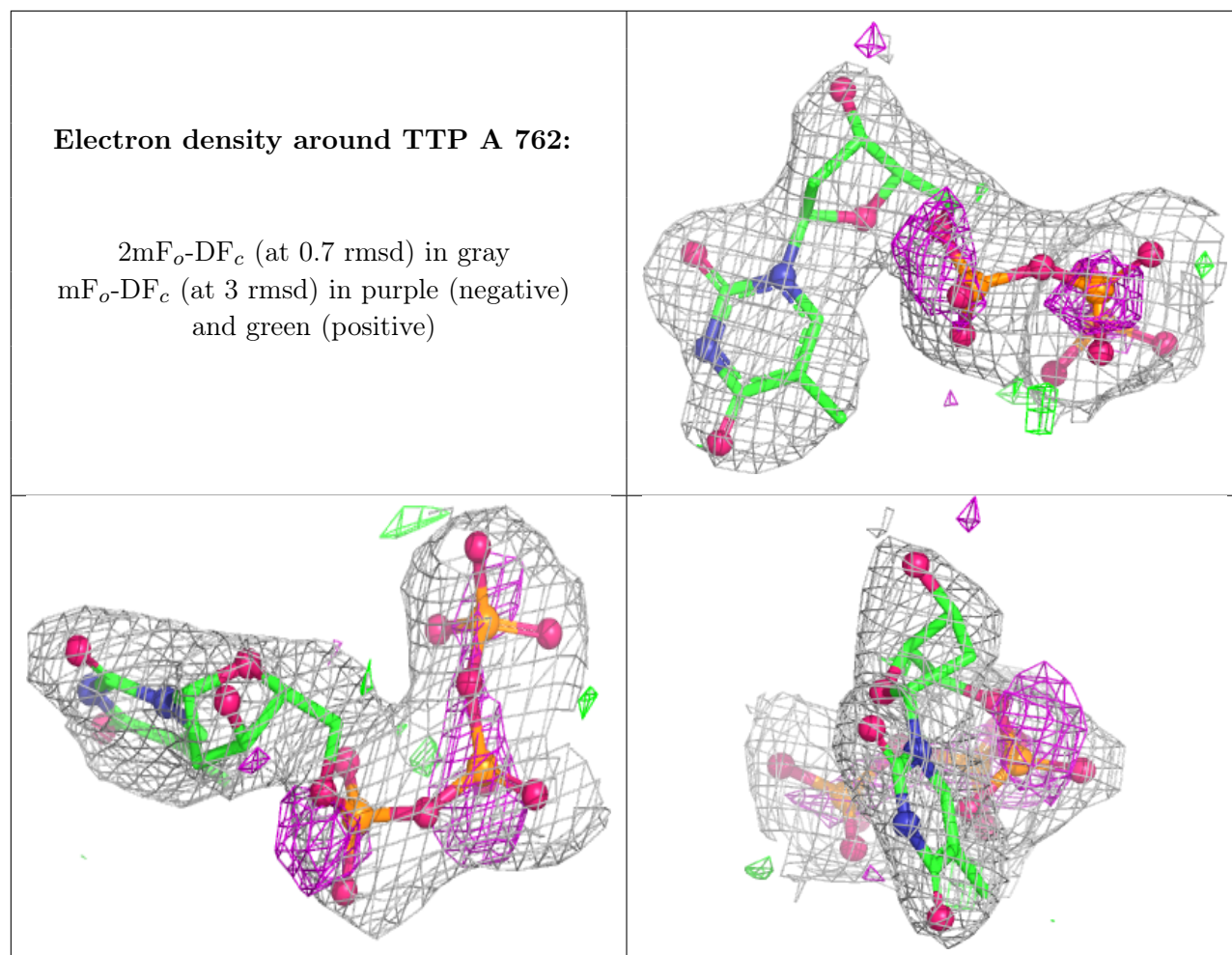
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.