



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:46 PM UTC

PDB ID : 4MKV / pdb_00004mkv
Title : Structure of Pisum sativum Rubisco with ABA
Authors : Loewen, M.C.; Loewen, P.C.; Switala, J.
Deposited on : 2013-09-05
Resolution : 2.15 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

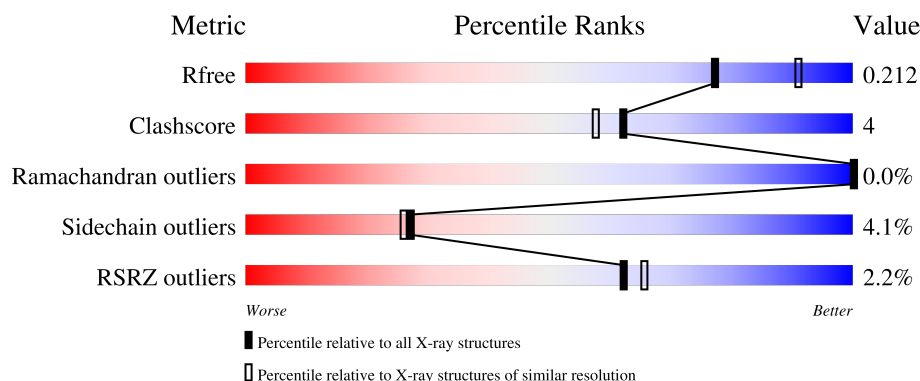
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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.



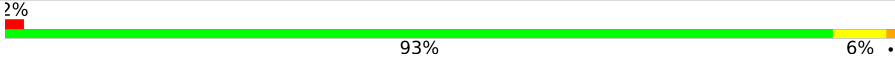
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	458	2% 86% 12%
1	B	458	2% 85% 14%
1	C	458	2% 84% 13%
1	D	458	2% 84% 14%
2	S	123	2% 88% 11%

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Mol	Chain	Length	Quality of chain
2	T	123	 2% 93% 6% .
2	U	123	 6% 89% 11% .
2	V	123	 6% 82% 17% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19725 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 Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	3	0
			3608	2299	632	660	17			
1	B	458	Total	C	N	O	S	0	4	0
			3609	2303	631	658	17			
1	C	458	Total	C	N	O	S	0	5	0
			3621	2309	635	660	17			
1	D	458	Total	C	N	O	S	0	5	0
			3619	2307	633	662	17			

- Molecule 2 is a protein called Ribulose biphosphate carboxylase small chain 3A, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	0	0
			1029	678	171	175	5			
2	T	123	Total	C	N	O	S	0	1	0
			1033	682	171	175	5			
2	U	123	Total	C	N	O	S	0	2	0
			1041	686	174	176	5			
2	V	123	Total	C	N	O	S	0	0	0
			1029	678	171	175	5			

There are 24 discrepancies between the modelled and reference sequences:

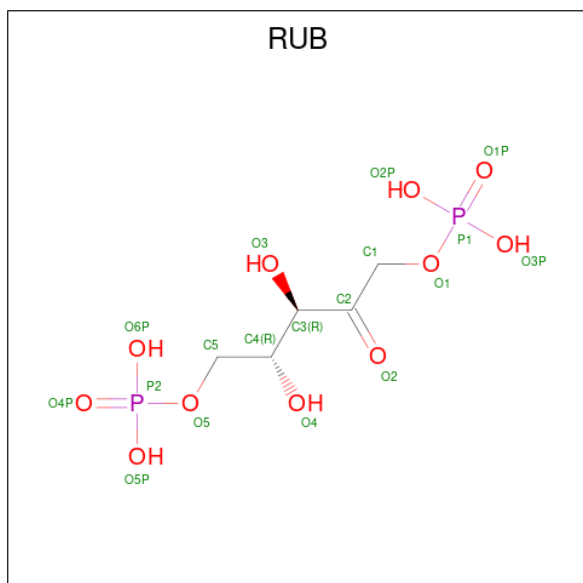
Chain	Residue	Modelled	Actual	Comment	Reference
S	47	LYS	GLU	conflict	UNP P07689
S	91	LYS	VAL	conflict	UNP P07689
S	92	LYS	ALA	conflict	UNP P07689
S	96	ARG	GLN	conflict	UNP P07689
S	121	ALA	GLU	conflict	UNP P07689
S	122	GLY	SER	conflict	UNP P07689
T	47	LYS	GLU	conflict	UNP P07689
T	91	LYS	VAL	conflict	UNP P07689

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Chain	Residue	Modelled	Actual	Comment	Reference
T	92	LYS	ALA	conflict	UNP P07689
T	96	ARG	GLN	conflict	UNP P07689
T	121	ALA	GLU	conflict	UNP P07689
T	122	GLY	SER	conflict	UNP P07689
U	47	LYS	GLU	conflict	UNP P07689
U	91	LYS	VAL	conflict	UNP P07689
U	92	LYS	ALA	conflict	UNP P07689
U	96	ARG	GLN	conflict	UNP P07689
U	121	ALA	GLU	conflict	UNP P07689
U	122	GLY	SER	conflict	UNP P07689
V	47	LYS	GLU	conflict	UNP P07689
V	91	LYS	VAL	conflict	UNP P07689
V	92	LYS	ALA	conflict	UNP P07689
V	96	ARG	GLN	conflict	UNP P07689
V	121	ALA	GLU	conflict	UNP P07689
V	122	GLY	SER	conflict	UNP P07689

- Molecule 3 is RIBULOSE-1,5-DIPHOSPHATE (CCD ID: RUB) (formula: $C_5H_{12}O_{11}P_2$).



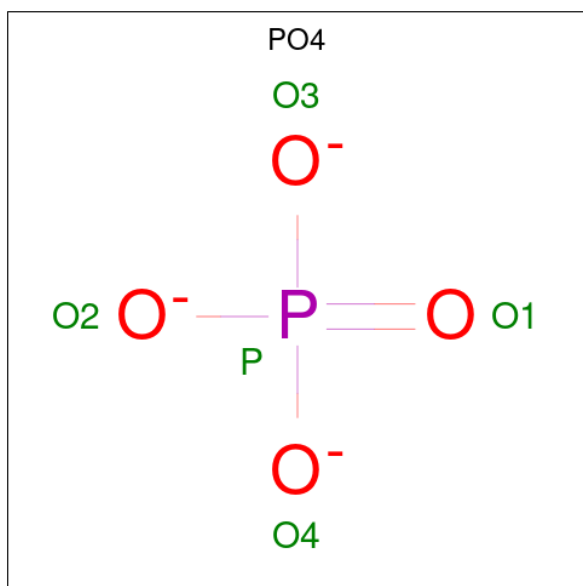
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			18	5	11	2		
3	B	1	Total	C	O	P	0	0
			18	5	11	2		
3	C	1	Total	C	O	P	0	0
			18	5	11	2		

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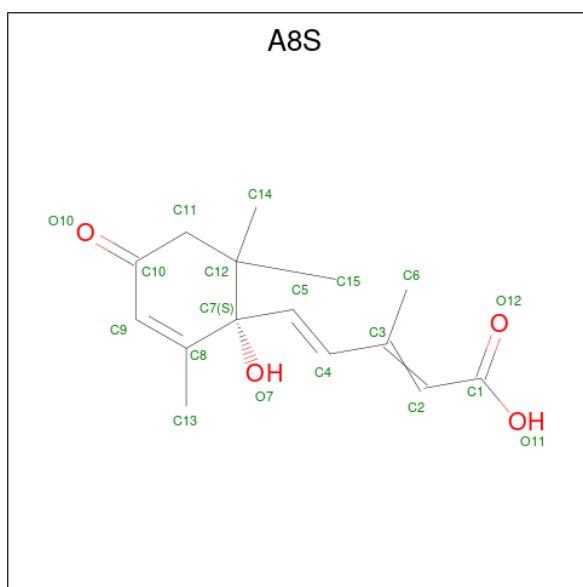
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	O	P	0	0
			18	5	11	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is (2Z,4E)-5-[(1S)-1-hydroxy-2,6,6-trimethyl-4-oxocyclohex-2-en-1-yl]-3-methylpenta-2,4-dienoic acid (CCD ID: A8S) (formula: $C_{15}H_{20}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			19	15	4		

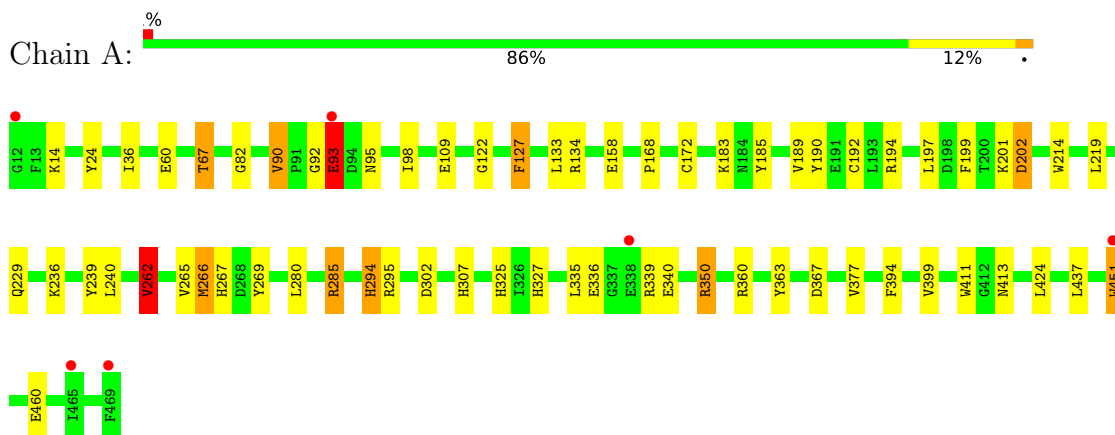
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	215	Total	O	0	0
			215	215		
6	B	208	Total	O	0	0
			208	208		
6	C	174	Total	O	0	0
			174	174		
6	D	201	Total	O	0	0
			201	201		
6	S	67	Total	O	0	0
			67	67		
6	T	77	Total	O	0	0
			77	77		
6	U	36	Total	O	0	0
			36	36		
6	V	52	Total	O	0	0
			52	52		

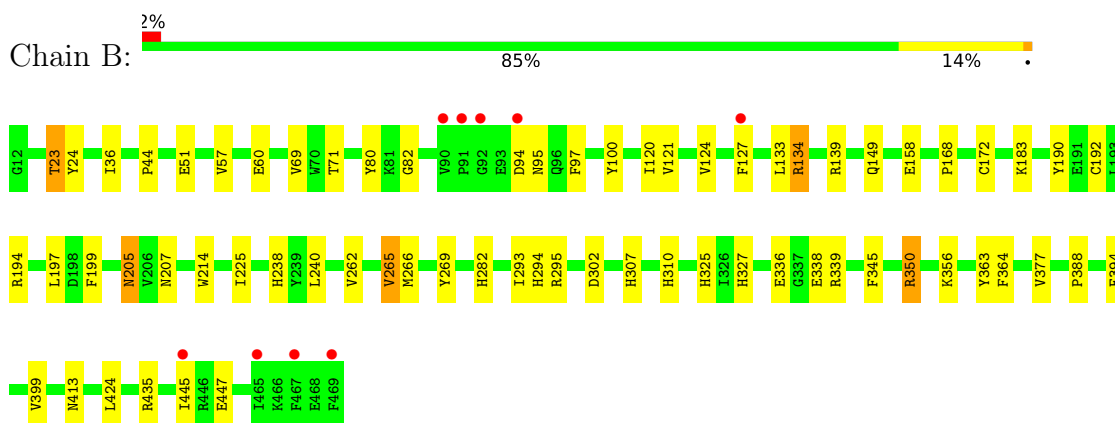
3 Residue-property plots [i](#)

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

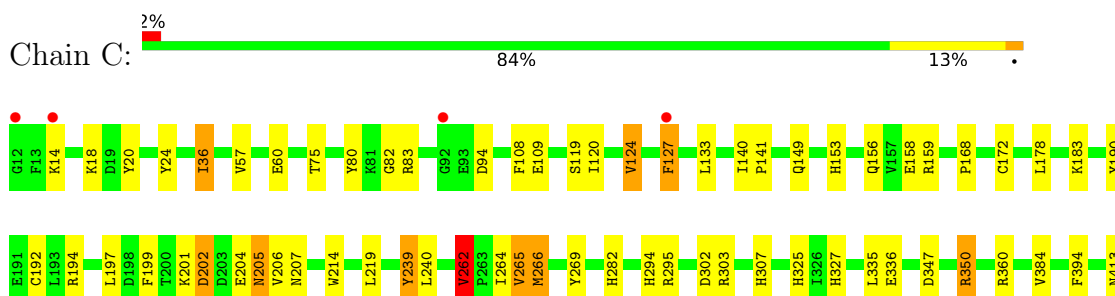
- Molecule 1: Ribulose biphosphate carboxylase large chain

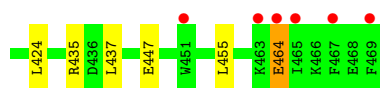


- Molecule 1: Ribulose biphosphate carboxylase large chain

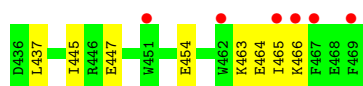
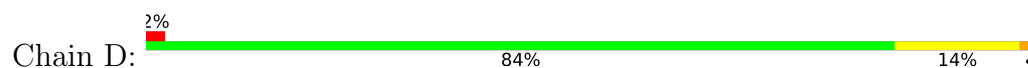


- Molecule 1: Ribulose biphosphate carboxylase large chain

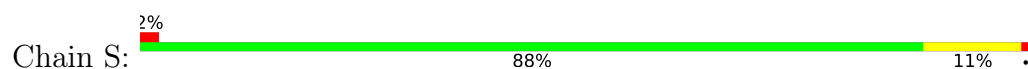




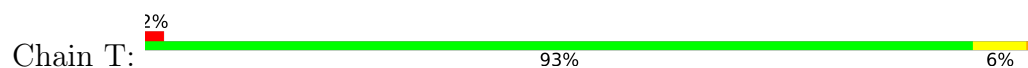
- Molecule 1: Ribulose biphosphate carboxylase large chain



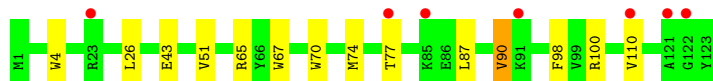
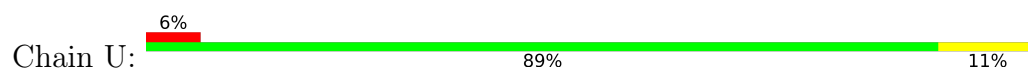
- Molecule 2: Ribulose biphosphate carboxylase small chain 3A, chloroplastic



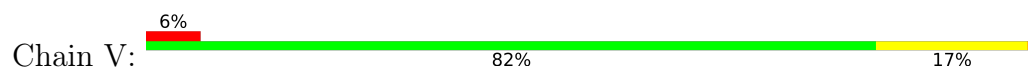
- Molecule 2: Ribulose biphosphate carboxylase small chain 3A, chloroplastic



- Molecule 2: Ribulose biphosphate carboxylase small chain 3A, chloroplastic



- Molecule 2: Ribulose biphosphate carboxylase small chain 3A, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	110.44Å 110.23Å 203.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.51 – 2.15 48.51 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.9 (48.51-2.15) 94.9 (48.51-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.16Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.162 , 0.197 0.174 , 0.212	Depositor DCC
R_{free} test set	6458 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.065 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19725	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.71% 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: A8S, PO4, RUB

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	0.87	2/3704 (0.1%)	1.27	17/5021 (0.3%)
1	B	0.88	0/3711	1.25	19/5031 (0.4%)
1	C	0.84	2/3728 (0.1%)	1.30	25/5053 (0.5%)
1	D	0.87	1/3723 (0.0%)	1.28	22/5047 (0.4%)
2	S	0.83	0/1062	1.13	2/1436 (0.1%)
2	T	0.83	0/1069	1.13	1/1446 (0.1%)
2	U	0.80	0/1080	1.14	1/1460 (0.1%)
2	V	0.83	1/1062 (0.1%)	1.22	6/1436 (0.4%)
All	All	0.86	6/19139 (0.0%)	1.25	93/25930 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	266	MET	SD-CE	-10.44	1.53	1.79
2	V	74	MET	SD-CE	-6.62	1.63	1.79
1	C	266	MET	SD-CE	-6.58	1.63	1.79
1	A	266	MET	SD-CE	-6.35	1.63	1.79
1	A	90	VAL	CA-C	5.36	1.58	1.52
1	C	140	ILE	CG1-CD1	-5.09	1.31	1.51

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	464	GLU	CA-C-N	8.00	133.14	122.90
1	C	464	GLU	C-N-CA	8.00	133.14	122.90
1	C	204	GLU	CA-C-N	7.82	132.19	120.31
1	C	204	GLU	C-N-CA	7.82	132.19	120.31
2	V	105	ASP	CA-C-N	7.79	131.05	120.38
2	V	105	ASP	C-N-CA	7.79	131.05	120.38
1	B	121	VAL	N-CA-CB	-7.52	102.39	112.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	262	VAL	N-CA-CB	-7.16	101.18	111.21
1	D	205	ASN	CA-CB-CG	7.15	119.75	112.60
1	C	82	GLY	N-CA-C	-7.10	102.43	112.37
1	B	82	GLY	N-CA-C	-6.73	102.94	112.37
1	C	302	ASP	N-CA-C	6.70	121.16	112.92
1	C	120	ILE	N-CA-C	6.68	116.83	110.42
1	A	202	ASP	CA-CB-CG	6.53	119.13	112.60
1	D	413	ASN	N-CA-C	6.52	118.04	111.07
1	C	413	ASN	N-CA-C	6.48	118.00	111.07
1	B	139	ARG	CA-C-N	-6.48	117.92	122.59
1	B	139	ARG	C-N-CA	-6.48	117.92	122.59
1	C	94	ASP	N-CA-C	6.43	119.04	109.59
1	C	269	TYR	N-CA-C	6.43	119.10	111.71
1	B	302	ASP	N-CA-C	6.38	121.22	113.17
1	A	82	GLY	N-CA-C	-6.36	103.47	112.37
1	C	262	VAL	N-CA-CB	-6.36	102.31	111.21
1	A	93	GLU	CA-C-N	6.34	133.11	121.70
1	A	93	GLU	C-N-CA	6.34	133.11	121.70
1	A	262	VAL	N-CA-CB	-6.28	102.42	111.21
1	D	82	GLY	N-CA-C	-6.27	103.59	112.37
1	D	302	ASP	N-CA-C	6.26	120.62	112.92
1	C	202	ASP	CA-CB-CG	6.24	118.84	112.60
1	B	269	TYR	N-CA-C	6.23	118.87	111.71
1	A	302	ASP	N-CA-C	6.22	120.57	112.92
1	D	204	GLU	CA-C-N	6.17	131.17	120.68
1	D	204	GLU	C-N-CA	6.17	131.17	120.68
1	C	20	TYR	CA-C-N	6.15	128.81	120.38
1	C	20	TYR	C-N-CA	6.15	128.81	120.38
1	D	264	ILE	N-CA-C	6.13	116.45	108.35
1	B	214	TRP	N-CA-C	6.10	117.59	111.07
1	A	214	TRP	N-CA-C	6.10	117.59	111.07
1	A	269	TYR	N-CA-C	6.06	118.68	111.71
1	A	413	ASN	N-CA-C	5.99	117.48	111.07
2	V	79	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	413	ASN	N-CA-C	5.82	117.30	111.07
2	S	98	PHE	N-CA-C	-5.76	100.28	109.96
1	D	80	TYR	N-CA-C	5.66	120.32	113.41
1	A	199	PHE	CA-CB-CG	5.64	119.44	113.80
1	C	350	ARG	CB-CG-CD	-5.61	98.40	111.30
1	A	350	ARG	CB-CG-CD	-5.61	98.40	111.30
1	C	214	TRP	N-CA-C	5.57	117.03	111.07
1	D	465	ILE	N-CA-C	5.57	115.58	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	ARG	CB-CG-CD	-5.55	98.54	111.30
1	D	350	ARG	CB-CG-CD	-5.54	98.55	111.30
2	T	98	PHE	N-CA-C	-5.52	100.68	109.96
1	B	199	PHE	CA-CB-CG	5.52	119.32	113.80
2	U	98	PHE	N-CA-C	-5.50	100.33	109.46
1	B	265	VAL	N-CA-CB	-5.50	104.82	112.52
1	C	109	GLU	CB-CG-CD	5.50	121.94	112.60
1	A	122	GLY	N-CA-C	5.48	118.86	112.50
1	C	199	PHE	CA-CB-CG	5.47	119.27	113.80
1	D	36	ILE	N-CA-C	-5.44	100.75	108.58
1	D	214	TRP	N-CA-C	5.43	116.88	111.07
1	D	293	ILE	N-CA-C	5.42	115.75	108.17
1	D	109	GLU	CB-CG-CD	5.38	121.74	112.60
1	C	36	ILE	N-CA-C	-5.33	100.90	108.58
1	C	264	ILE	N-CA-C	5.32	116.33	108.45
1	C	265	VAL	CB-CA-C	5.32	118.48	111.19
1	A	109	GLU	CB-CG-CD	5.32	121.64	112.60
2	S	102	ILE	CA-CB-CG2	5.29	119.49	110.50
1	D	339	ARG	N-CA-C	5.27	117.45	111.02
1	B	80	TYR	N-CA-C	5.27	119.84	113.41
2	V	14	THR	CB-CA-C	5.26	116.27	109.80
1	D	384	VAL	N-CA-C	5.25	116.60	110.62
2	V	98	PHE	N-CA-C	-5.25	100.75	109.46
1	D	199	PHE	CA-CB-CG	5.23	119.03	113.80
1	B	24	TYR	N-CA-C	5.21	119.79	113.38
1	B	345	PHE	CA-CB-CG	5.20	119.00	113.80
1	B	293	ILE	N-CA-C	5.19	115.43	108.17
1	A	36	ILE	N-CA-C	-5.18	101.12	108.58
1	D	269	TYR	N-CA-C	5.18	117.67	111.71
1	B	120	ILE	N-CA-C	5.18	115.90	110.62
1	C	80	TYR	N-CA-C	5.16	119.70	113.41
1	C	265	VAL	N-CA-CB	-5.14	105.96	112.60
1	B	339	ARG	N-CA-C	5.13	117.28	111.02
1	A	24	TYR	N-CA-C	5.13	119.69	113.38
1	D	248	GLU	CB-CG-CD	5.12	121.30	112.60
1	C	24	TYR	N-CA-C	5.11	119.66	113.38
1	B	207	ASN	CA-CB-CG	5.08	117.68	112.60
1	D	24	TYR	N-CA-C	5.08	119.63	113.38
1	D	108	PHE	N-CA-C	5.07	118.07	109.76
1	B	36	ILE	N-CA-C	-5.05	101.31	108.58
1	A	90	VAL	N-CA-CB	-5.03	104.17	111.21
2	V	106	ASN	N-CA-CB	-5.02	102.53	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	PHE	N-CA-C	5.02	117.99	109.76
1	A	67	THR	CB-CA-C	-5.00	99.53	109.79

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	3608	0	3545	31	0
1	B	3609	0	3557	36	0
1	C	3621	0	3561	31	1
1	D	3619	0	3552	31	1
2	S	1029	0	1037	8	0
2	T	1033	0	1046	3	0
2	U	1041	0	1057	5	0
2	V	1029	0	1037	9	0
3	A	18	0	8	1	0
3	B	18	0	8	0	0
3	C	18	0	8	1	0
3	D	18	0	8	1	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	B	19	0	19	5	0
6	A	215	0	0	3	0
6	B	208	0	0	1	0
6	C	174	0	0	2	0
6	D	201	0	0	0	0
6	S	67	0	0	3	0
6	T	77	0	0	0	0
6	U	36	0	0	0	0
6	V	52	0	0	2	0
All	All	19725	0	18443	151	1

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 4.

All (151) 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:D:239:TYR:HB2	1:D:266:MET:HE2	1.48	0.95
1:C:60:GLU:HG3	1:C:127:PHE:HZ	1.35	0.86
2:S:55:HIS:HD2	6:S:266:HOH:O	1.57	0.86
1:B:266:MET:HE3	1:B:294:HIS:HD2	1.40	0.83
1:C:60:GLU:HG3	1:C:127:PHE:CZ	2.13	0.82
1:A:60:GLU:HG3	1:A:127:PHE:HZ	1.47	0.79
1:D:409:HIS:HD2	1:D:411:TRP:H	1.30	0.78
1:D:178:LEU:HD21	1:D:205:ASN:HB3	1.67	0.76
2:U:74:MET:HE2	2:U:77:THR:HG21	1.69	0.75
1:D:409:HIS:CD2	1:D:411:TRP:H	2.07	0.72
2:T:67:TRP:CZ3	2:T:100:ARG:HG3	2.27	0.70
1:A:367:ASP:OD1	6:A:814:HOH:O	2.10	0.70
1:C:194:ARG:NH2	2:U:4:TRP:O	2.25	0.69
2:U:67:TRP:CZ3	2:U:100:ARG:HG3	2.28	0.68
2:V:67:TRP:CZ3	2:V:100:ARG:HG3	2.27	0.68
1:A:60:GLU:HG3	1:A:127:PHE:CZ	2.27	0.68
2:S:67:TRP:CZ3	2:S:100:ARG:HG3	2.28	0.68
1:B:266:MET:CE	1:B:294:HIS:HD2	2.09	0.65
1:C:178:LEU:HD21	1:C:205:ASN:HB3	1.79	0.65
1:B:363:TYR:O	5:B:502:A8S:H13A	1.98	0.63
1:B:69[A]:VAL:HG12	1:B:71:THR:OG1	2.00	0.62
1:D:388:PRO:HD3	1:D:445:ILE:HD11	1.82	0.61
1:C:350:ARG:NH2	1:C:394:PHE:O	2.33	0.61
1:D:350:ARG:NH2	1:D:394:PHE:O	2.30	0.61
2:V:43:GLU:OE1	2:V:100:ARG:NH1	2.33	0.61
1:C:57:VAL:HA	1:C:124:VAL:HG21	1.84	0.59
1:A:202:ASP:HB2	1:A:266:MET:HE1	1.84	0.59
2:U:43:GLU:OE1	2:U:100:ARG:NH1	2.35	0.59
1:A:335:LEU:CD1	3:A:501:RUB:H52	2.33	0.59
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.87	0.58
1:B:57:VAL:HA	1:B:124:VAL:HG21	1.86	0.58
1:A:93:GLU:HA	1:A:95:ASN:H	1.68	0.58
1:B:350:ARG:NH2	1:B:394:PHE:O	2.34	0.57
1:B:205:ASN:H	1:B:205:ASN:HD22	1.53	0.56
1:D:335:LEU:CD1	3:D:501:RUB:H52	2.35	0.56
1:C:57:VAL:HA	1:C:124:VAL:CG2	2.35	0.56
1:D:201:LYS:HB2	1:D:266:MET:HE1	1.88	0.56
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:TRP:HD1	6:S:251:HOH:O	1.90	0.55
1:D:201:LYS:HB3	1:D:239:TYR:CD2	2.41	0.55
1:B:100:TYR:CE1	5:B:502:A8S:H13	2.42	0.55
1:A:168:PRO:HD2	1:A:424:LEU:HD11	1.89	0.55
1:B:356:LYS:HD2	5:B:502:A8S:H6	1.88	0.54
2:V:100:ARG:NH2	6:V:224:HOH:O	2.40	0.54
1:A:350:ARG:NH2	1:A:394:PHE:O	2.35	0.54
1:C:149:GLN:HE22	1:C:282:HIS:HA	1.72	0.53
1:B:266:MET:CE	1:B:294:HIS:CD2	2.90	0.53
1:B:168:PRO:HD2	1:B:424:LEU:HD11	1.92	0.52
1:B:364:PHE:HE1	5:B:502:A8S:H9	1.75	0.52
1:C:202:ASP:HB2	1:C:266:MET:HE1	1.90	0.52
1:D:158:GLU:CD	1:D:325:HIS:HE2	2.16	0.52
1:C:335:LEU:CD1	3:C:501:RUB:H52	2.40	0.51
1:C:347:ASP:OD2	1:C:360:ARG:NH2	2.42	0.51
1:C:168:PRO:HD2	1:C:424:LEU:HD11	1.92	0.51
1:C:384:VAL:HG11	1:C:455:LEU:HD11	1.94	0.50
2:S:74:MET:HE2	6:S:245:HOH:O	2.11	0.50
1:D:168:PRO:HD2	1:D:424:LEU:HD11	1.93	0.50
2:T:51[A]:VAL:HG13	2:T:62:TYR:HB3	1.92	0.50
1:A:201:LYS:NZ	1:A:294:HIS:NE2	2.52	0.50
1:A:98:ILE:HD13	1:A:363:TYR:HE2	1.77	0.49
1:C:190:TYR:CZ	1:C:194:ARG:HD2	2.47	0.49
1:B:388:PRO:HD3	1:B:445:ILE:HD11	1.93	0.49
1:B:69[A]:VAL:CG1	1:B:71:THR:OG1	2.61	0.49
1:D:292:HIS:HD2	1:D:325:HIS:ND1	2.11	0.48
1:A:158:GLU:CD	1:A:325:HIS:HE2	2.20	0.48
1:C:435:ARG:NH2	1:C:447:GLU:OE1	2.46	0.48
1:C:206:VAL:C	1:C:207:ASN:HD22	2.22	0.48
2:S:100:ARG:HD2	2:S:102:ILE:HD11	1.96	0.47
1:A:201:LYS:HB3	1:A:239:TYR:CD2	2.49	0.47
1:C:158:GLU:CD	1:C:325:HIS:HE2	2.23	0.47
2:U:70:TRP:CE3	2:U:90:VAL:HG13	2.49	0.47
1:C:192:CYS:HB3	1:C:197:LEU:HD12	1.97	0.47
1:C:201:LYS:HB3	1:C:239:TYR:CD2	2.49	0.47
1:B:158:GLU:CD	1:B:325:HIS:HE2	2.19	0.47
1:B:205:ASN:H	1:B:205:ASN:ND2	2.12	0.47
1:B:192:CYS:HB3	1:B:197:LEU:HD12	1.97	0.46
2:V:35:ARG:HD2	6:V:241:HOH:O	2.13	0.46
2:V:100:ARG:HD2	2:V:102:ILE:HD11	1.97	0.46
1:A:192:CYS:HB3	1:A:197:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:TYR:OH	1:D:202:ASP:HA	2.15	0.46
1:D:44:PRO:HG2	1:D:95:ASN:HD22	1.81	0.46
2:V:102:ILE:HG12	2:V:111:GLN:NE2	2.31	0.46
1:A:229:GLN:HE21	1:A:236:LYS:H	1.63	0.45
1:C:384:VAL:CG1	1:C:455:LEU:HD11	2.46	0.45
1:B:44:PRO:HG3	1:B:97:PHE:HE1	1.81	0.45
1:D:192:CYS:HB3	1:D:197:LEU:HD12	1.99	0.45
1:B:57:VAL:HA	1:B:124:VAL:CG2	2.46	0.45
1:B:133:LEU:H	1:B:307:HIS:CD2	2.35	0.45
1:D:240:LEU:HD12	1:D:262:VAL:HG11	1.98	0.45
2:S:102:ILE:HG12	2:S:111:GLN:NE2	2.32	0.45
1:B:205:ASN:HD22	1:B:205:ASN:N	2.15	0.45
1:B:149:GLN:HE22	1:B:282:HIS:HA	1.81	0.44
1:A:172:CYS:HB3	1:A:197:LEU:HD13	1.98	0.44
1:A:340:GLU:O	1:A:360:ARG:HG2	2.17	0.44
1:C:159:ARG:NH2	6:C:720:HOH:O	2.51	0.44
1:A:92:GLY:O	1:A:93:GLU:HB2	2.18	0.44
1:B:266:MET:HE3	1:B:294:HIS:CD2	2.32	0.44
2:S:70:TRP:CD2	2:S:90:VAL:HG22	2.53	0.44
1:A:133:LEU:H	1:A:307:HIS:CD2	2.36	0.44
1:A:267:HIS:HB2	1:A:280:LEU:HD23	2.00	0.44
1:B:94:ASP:HA	1:B:95:ASN:HA	1.67	0.44
1:A:339:ARG:NH1	6:A:753:HOH:O	2.39	0.44
1:A:295:ARG:HG2	1:A:327:HIS:HB2	1.99	0.44
1:A:240:LEU:HD12	1:A:262:VAL:HG11	2.00	0.43
1:B:134:ARG:NH2	1:B:310:HIS:HD2	2.15	0.43
1:B:190:TYR:CZ	1:B:194:ARG:HD3	2.53	0.43
2:S:46:LEU:HD13	2:T:7:ILE:HD12	2.00	0.43
1:B:172:CYS:HB3	1:B:197:LEU:HD13	2.00	0.43
1:A:185:TYR:O	1:A:189:VAL:HG23	2.18	0.43
1:B:100:TYR:CE1	5:B:502:A8S:C13	3.02	0.43
1:B:435:ARG:NH2	1:B:447:GLU:OE1	2.49	0.43
1:C:384:VAL:HG11	1:C:455:LEU:CD1	2.49	0.43
1:C:295:ARG:HG2	1:C:327:HIS:HB2	2.00	0.42
1:D:295:ARG:HG2	1:D:327:HIS:HB2	2.01	0.42
1:A:411:TRP:CZ3	2:S:2:GLN:HB2	2.54	0.42
1:D:75:THR:HG22	1:D:76[A]:SER:H	1.83	0.42
1:A:172:CYS:CB	1:A:197:LEU:HD13	2.49	0.42
1:D:225:ILE:HD11	1:D:238:HIS:HB3	2.01	0.42
1:D:75:THR:HG22	1:D:76[B]:SER:H	1.83	0.42
1:C:239:TYR:HB2	1:C:266:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:CYS:HB3	1:C:197:LEU:HD13	2.00	0.42
1:B:23:THR:CG2	6:B:671:HOH:O	2.68	0.42
1:C:153:HIS:HE1	6:C:612:HOH:O	2.02	0.42
1:B:172:CYS:CB	1:B:197:LEU:HD13	2.50	0.41
1:B:240:LEU:HD12	1:B:262:VAL:HG21	2.02	0.41
1:C:172:CYS:CB	1:C:197:LEU:HD13	2.50	0.41
1:A:133:LEU:H	1:A:307:HIS:HD2	1.68	0.41
1:B:377:VAL:HG22	1:B:399:VAL:HB	2.03	0.41
1:C:133:LEU:H	1:C:307:HIS:CD2	2.37	0.41
1:D:409:HIS:HE1	1:D:454:GLU:O	2.03	0.41
2:V:69:MET:HE3	2:V:71:LYS:O	2.20	0.41
1:B:295:ARG:HG2	1:B:327:HIS:HB2	2.01	0.41
1:D:36:ILE:HG12	1:D:141:PRO:CD	2.50	0.41
1:C:240:LEU:HD12	1:C:262:VAL:HG11	2.03	0.41
2:V:97:ALA:O	2:V:118:HIS:HD2	2.03	0.41
1:B:57:VAL:HG13	1:B:124:VAL:HG21	2.01	0.41
1:B:225:ILE:HD11	1:B:238:HIS:HB3	2.03	0.41
1:D:377:VAL:HG22	1:D:399:VAL:HB	2.02	0.41
1:D:172:CYS:CB	1:D:197:LEU:HD13	2.52	0.41
1:D:185:TYR:O	1:D:189:VAL:HG23	2.21	0.41
1:C:36:ILE:HG12	1:C:141:PRO:CD	2.51	0.40
1:D:172:CYS:HB3	1:D:197:LEU:HD13	2.01	0.40
1:D:435:ARG:NH2	1:D:447:GLU:OE1	2.48	0.40
1:A:285:ARG:NH2	6:A:803:HOH:O	2.53	0.40
1:D:357:ASP:OD2	1:D:360:ARG:HD3	2.21	0.40
1:A:266:MET:HE2	1:A:266:MET:HB3	1.82	0.40
1:A:377:VAL:HG22	1:A:399:VAL:HB	2.03	0.40
1:D:190:TYR:CZ	1:D:194:ARG:HD3	2.56	0.40
1:A:190:TYR:CZ	1:A:194:ARG:HD3	2.56	0.40
2:V:23:ARG:HE	2:V:84:LEU:HD13	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ARG:NH2	1:D:127:PHE:O[2_555]	2.19	0.01

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	459/458 (100%)	443 (96%)	15 (3%)	1 (0%)	43	44
1	B	460/458 (100%)	441 (96%)	19 (4%)	0	100	100
1	C	461/458 (101%)	445 (96%)	16 (4%)	0	100	100
1	D	461/458 (101%)	444 (96%)	17 (4%)	0	100	100
2	S	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
2	T	122/123 (99%)	119 (98%)	3 (2%)	0	100	100
2	U	123/123 (100%)	120 (98%)	3 (2%)	0	100	100
2	V	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
All	All	2328/2324 (100%)	2248 (97%)	79 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	GLU

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	373/370 (101%)	356 (95%)	17 (5%)	24	22
1	B	374/370 (101%)	364 (97%)	10 (3%)	39	41
1	C	375/370 (101%)	356 (95%)	19 (5%)	21	18
1	D	375/370 (101%)	359 (96%)	16 (4%)	26	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	110/110 (100%)	105 (96%)	5 (4%)	24	22
2	T	111/110 (101%)	108 (97%)	3 (3%)	39	41
2	U	112/110 (102%)	106 (95%)	6 (5%)	20	16
2	V	110/110 (100%)	105 (96%)	5 (4%)	24	22
All	All	1940/1920 (101%)	1859 (96%)	81 (4%)	27	25

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	67	THR
1	A	90	VAL
1	A	93	GLU
1	A	127	PHE
1	A	134	ARG
1	A	183	LYS
1	A	219[A]	LEU
1	A	219[B]	LEU
1	A	262	VAL
1	A	265	VAL
1	A	285	ARG
1	A	294	HIS
1	A	336	GLU
1	A	437	LEU
1	A	451	TRP
1	A	460	GLU
1	B	23	THR
1	B	51	GLU
1	B	60	GLU
1	B	127	PHE
1	B	134	ARG
1	B	183	LYS
1	B	205	ASN
1	B	265	VAL
1	B	336	GLU
1	B	338	GLU
1	C	14	LYS
1	C	18	LYS
1	C	75	THR
1	C	83[A]	ARG
1	C	83[B]	ARG

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Mol	Chain	Res	Type
1	C	119[A]	SER
1	C	119[B]	SER
1	C	124	VAL
1	C	127	PHE
1	C	156	GLN
1	C	183	LYS
1	C	205	ASN
1	C	219	LEU
1	C	239	TYR
1	C	262	VAL
1	C	265	VAL
1	C	294	HIS
1	C	336	GLU
1	C	437	LEU
1	D	18	LYS
1	D	60	GLU
1	D	75	THR
1	D	93	GLU
1	D	127	PHE
1	D	175	LYS
1	D	183	LYS
1	D	239	TYR
1	D	262	VAL
1	D	294	HIS
1	D	336	GLU
1	D	384	VAL
1	D	437	LEU
1	D	463	LYS
1	D	464	GLU
1	D	466	LYS
2	S	26	LEU
2	S	51	VAL
2	S	65	ARG
2	S	87	LEU
2	S	102	ILE
2	T	7	ILE
2	T	87	LEU
2	T	92	LYS
2	U	26	LEU
2	U	51	VAL
2	U	65	ARG
2	U	87	LEU

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Mol	Chain	Res	Type
2	U	90	VAL
2	U	110	VAL
2	V	51	VAL
2	V	65	ARG
2	V	87	LEU
2	V	102	ILE
2	V	110	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	123	ASN
1	A	153	HIS
1	A	229	GLN
1	A	282	HIS
1	A	292	HIS
1	A	307	HIS
1	A	401	GLN
1	A	429	GLN
1	B	45	GLN
1	B	149	GLN
1	B	205	ASN
1	B	282	HIS
1	B	304	GLN
1	B	307	HIS
1	B	401	GLN
1	C	45	GLN
1	C	96	GLN
1	C	123	ASN
1	C	149	GLN
1	C	153	HIS
1	C	156	GLN
1	C	207	ASN
1	C	229	GLN
1	C	282	HIS
1	C	307	HIS
1	C	401	GLN
1	D	45	GLN
1	D	95	ASN
1	D	123	ASN
1	D	238	HIS

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Mol	Chain	Res	Type
1	D	282	HIS
1	D	292	HIS
1	D	307	HIS
1	D	401	GLN
1	D	409	HIS
2	S	2	GLN
2	S	55	HIS
2	S	118	HIS
2	U	2	GLN
2	U	55	HIS
2	U	118	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	C	502	-	4,4,4	0.87	0	6,6,6	0.75	0
3	RUB	C	501	-	17,17,17	3.94	6 (35%)	17,25,25	1.34	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	RUB	D	501	-	17,17,17	4.06	5 (29%)	17,25,25	1.57	4 (23%)
4	PO4	D	502	-	4,4,4	0.89	0	6,6,6	0.53	0
3	RUB	B	501	-	17,17,17	3.86	5 (29%)	17,25,25	1.26	1 (5%)
3	RUB	A	501	-	17,17,17	3.95	6 (35%)	17,25,25	1.53	2 (11%)
4	PO4	A	502	-	4,4,4	1.04	0	6,6,6	0.65	0
5	A8S	B	502	-	17,19,19	2.05	5 (29%)	17,29,29	1.97	5 (29%)

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	RUB	C	501	-	-	16/20/20/20	-
3	RUB	D	501	-	-	9/20/20/20	-
3	RUB	B	501	-	-	9/20/20/20	-
3	RUB	A	501	-	-	16/20/20/20	-
5	A8S	B	502	-	-	5/10/34/34	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	RUB	O2-C2	14.91	1.46	1.21
3	B	501	RUB	O2-C2	14.44	1.45	1.21
3	C	501	RUB	O2-C2	14.42	1.45	1.21
3	A	501	RUB	O2-C2	14.12	1.44	1.21
3	A	501	RUB	O1-C1	5.24	1.48	1.43
5	B	502	A8S	O12-C1	5.05	1.35	1.23
3	D	501	RUB	O1-C1	4.95	1.48	1.43
3	C	501	RUB	C5-C4	-3.84	1.46	1.51
3	C	501	RUB	O1-C1	3.58	1.47	1.43
3	B	501	RUB	O1-C1	3.35	1.46	1.43
3	B	501	RUB	C4-C3	-3.34	1.49	1.53
5	B	502	A8S	C7-C12	3.11	1.61	1.57
5	B	502	A8S	O11-C1	-2.97	1.22	1.30
3	A	501	RUB	C1-C2	-2.88	1.47	1.51
3	C	501	RUB	C4-C3	-2.66	1.49	1.53
3	A	501	RUB	C4-C3	-2.54	1.50	1.53
3	A	501	RUB	C5-C4	-2.53	1.48	1.51
3	D	501	RUB	C4-C3	-2.51	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	A8S	C4-C5	2.51	1.38	1.32
3	D	501	RUB	C1-C2	-2.50	1.47	1.51
3	B	501	RUB	C5-C4	-2.44	1.48	1.51
3	B	501	RUB	C1-C2	-2.42	1.47	1.51
3	A	501	RUB	P2-O5	2.38	1.67	1.60
3	C	501	RUB	C1-C2	-2.33	1.47	1.51
3	D	501	RUB	C5-C4	-2.32	1.48	1.51
5	B	502	A8S	C4-C3	2.21	1.50	1.46
3	C	501	RUB	P2-O5	2.13	1.67	1.60

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	A8S	O11-C1-C2	4.80	127.67	113.40
3	D	501	RUB	O5-C5-C4	4.00	120.04	109.36
3	B	501	RUB	O4-C4-C3	-3.85	104.09	109.67
3	A	501	RUB	O5-P2-O4P	3.43	115.72	106.44
5	B	502	A8S	O11-C1-O12	-3.21	116.17	122.70
3	C	501	RUB	O5-P2-O4P	2.67	113.64	106.44
3	D	501	RUB	O5-P2-O4P	2.66	113.64	106.44
5	B	502	A8S	O12-C1-C2	-2.60	116.07	124.02
3	C	501	RUB	O6P-P2-O5	-2.37	100.49	106.67
5	B	502	A8S	C4-C3-C2	2.36	125.68	119.15
3	D	501	RUB	O3-C3-C4	2.13	114.89	109.46
3	D	501	RUB	O6P-P2-O5	-2.07	101.27	106.67
3	A	501	RUB	O6P-P2-O5	-2.06	101.29	106.67
5	B	502	A8S	O7-C7-C12	-2.06	104.89	109.72

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	RUB	O1-C1-C2-C3
3	A	501	RUB	O1-C1-C2-O2
3	A	501	RUB	C1-C2-C3-C4
3	A	501	RUB	O2-C2-C3-C4
3	A	501	RUB	C2-C3-C4-C5
3	A	501	RUB	C2-C3-C4-O4
3	A	501	RUB	O3-C3-C4-C5
3	A	501	RUB	O3-C3-C4-O4
3	A	501	RUB	C1-O1-P1-O1P
3	A	501	RUB	C1-O1-P1-O2P

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Mol	Chain	Res	Type	Atoms
3	A	501	RUB	C1-O1-P1-O3P
3	A	501	RUB	C5-O5-P2-O5P
3	A	501	RUB	C5-O5-P2-O6P
3	B	501	RUB	O1-C1-C2-C3
3	B	501	RUB	O1-C1-C2-O2
3	B	501	RUB	C2-C3-C4-C5
3	B	501	RUB	C2-C3-C4-O4
3	B	501	RUB	O3-C3-C4-C5
3	B	501	RUB	O3-C3-C4-O4
3	B	501	RUB	C1-O1-P1-O2P
3	B	501	RUB	C1-O1-P1-O3P
3	C	501	RUB	O1-C1-C2-C3
3	C	501	RUB	O1-C1-C2-O2
3	C	501	RUB	C1-C2-C3-C4
3	C	501	RUB	O2-C2-C3-C4
3	C	501	RUB	C2-C3-C4-C5
3	C	501	RUB	C2-C3-C4-O4
3	C	501	RUB	O3-C3-C4-C5
3	C	501	RUB	O3-C3-C4-O4
3	C	501	RUB	C3-C4-C5-O5
3	C	501	RUB	C1-O1-P1-O2P
3	C	501	RUB	C1-O1-P1-O3P
3	C	501	RUB	C5-O5-P2-O5P
3	C	501	RUB	C5-O5-P2-O6P
3	D	501	RUB	C2-C3-C4-C5
3	D	501	RUB	C2-C3-C4-O4
3	D	501	RUB	O3-C3-C4-C5
3	D	501	RUB	O3-C3-C4-O4
3	D	501	RUB	C3-C4-C5-O5
3	D	501	RUB	C4-C5-O5-P2
5	B	502	A8S	C6-C3-C4-C5
5	B	502	A8S	C2-C3-C4-C5
3	B	501	RUB	C1-O1-P1-O1P
3	C	501	RUB	C1-O1-P1-O1P
3	D	501	RUB	O2-C2-C3-O3
3	A	501	RUB	C3-C4-C5-O5
5	B	502	A8S	C4-C5-C7-O7
3	A	501	RUB	O4-C4-C5-O5
3	C	501	RUB	C4-C5-O5-P2
5	B	502	A8S	O11-C1-C2-C3
5	B	502	A8S	O12-C1-C2-C3
3	A	501	RUB	C4-C5-O5-P2

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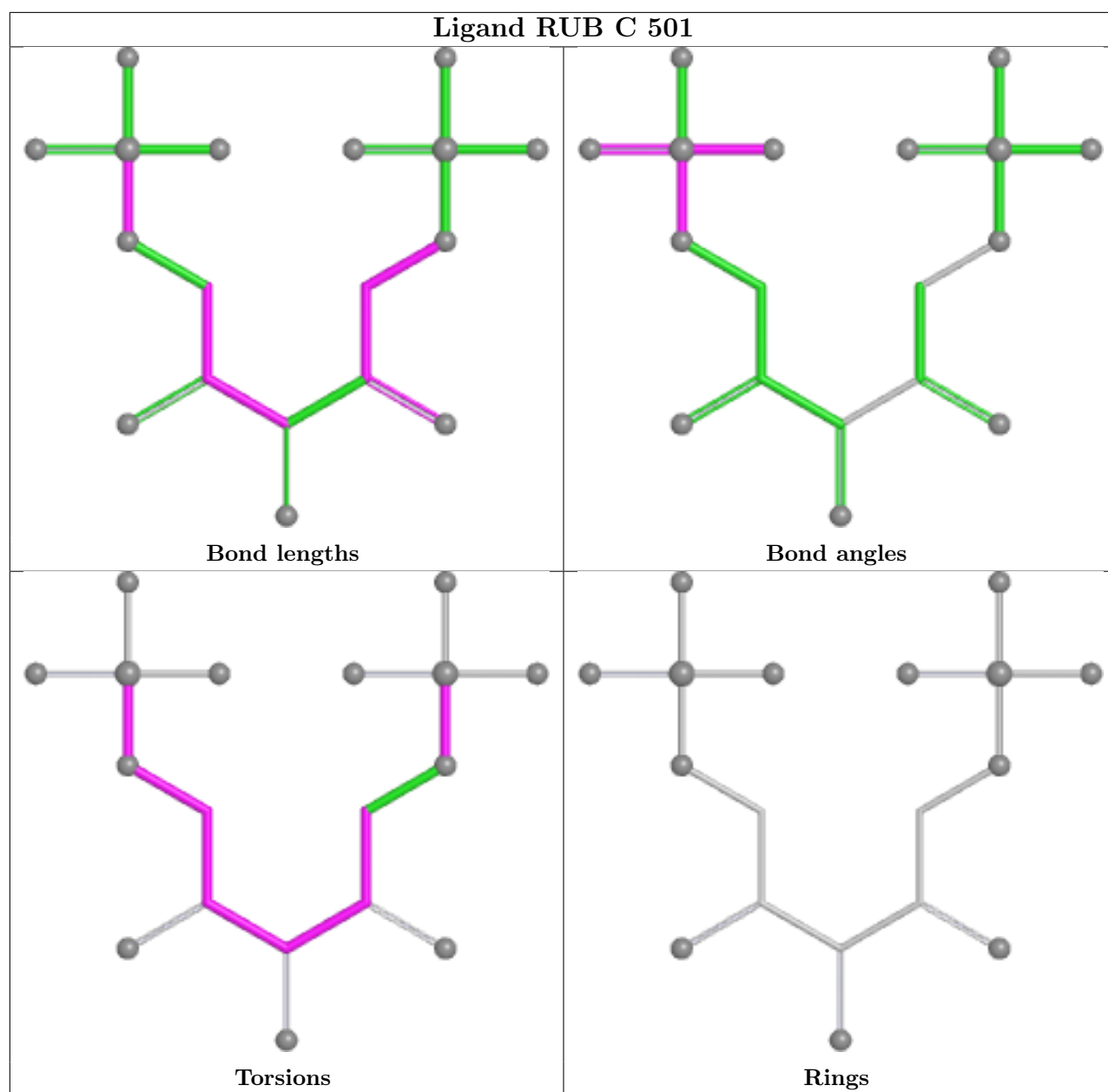
Mol	Chain	Res	Type	Atoms
3	C	501	RUB	O4-C4-C5-O5
3	D	501	RUB	O4-C4-C5-O5
3	D	501	RUB	C1-C2-C3-O3

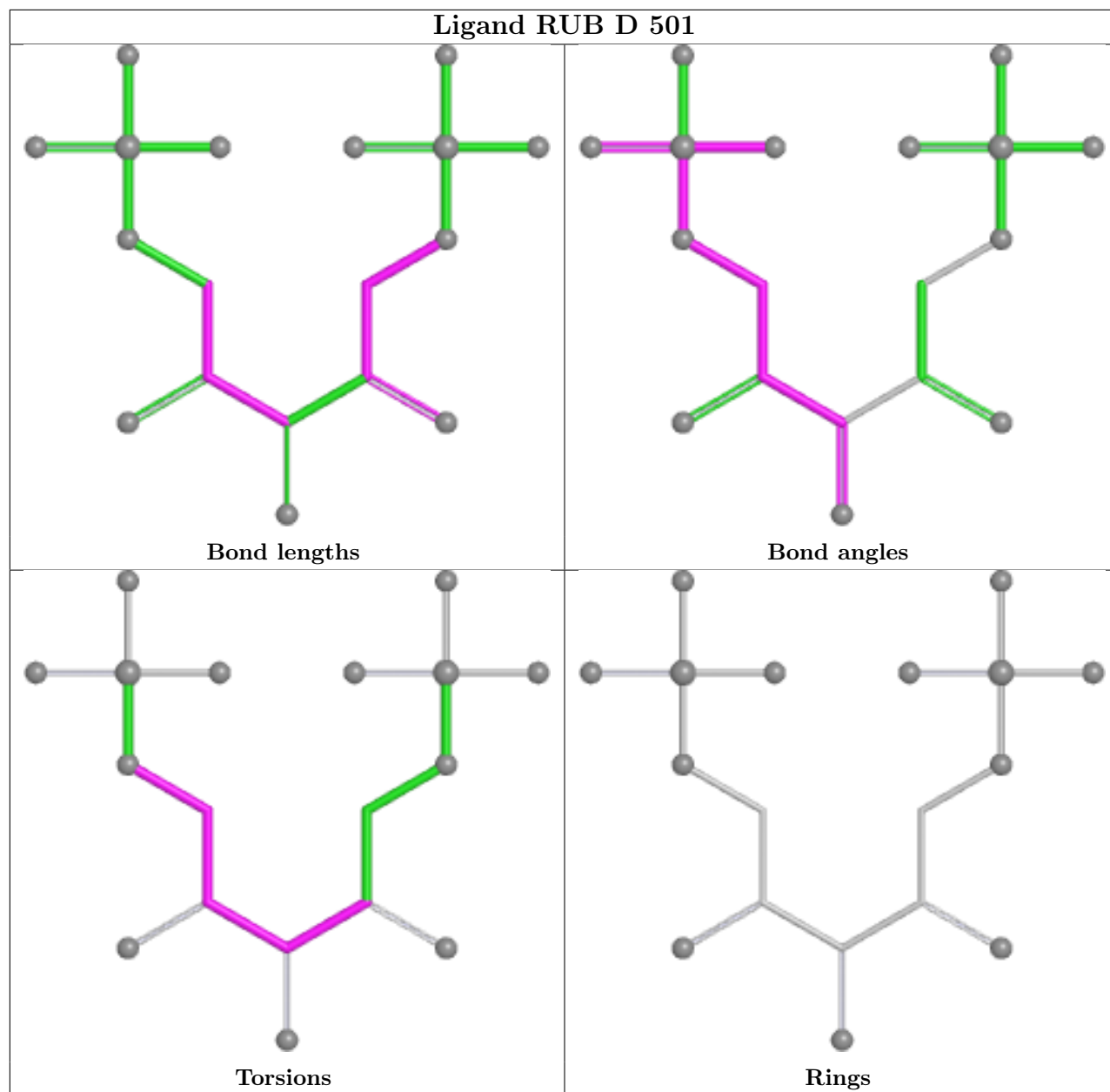
There are no ring outliers.

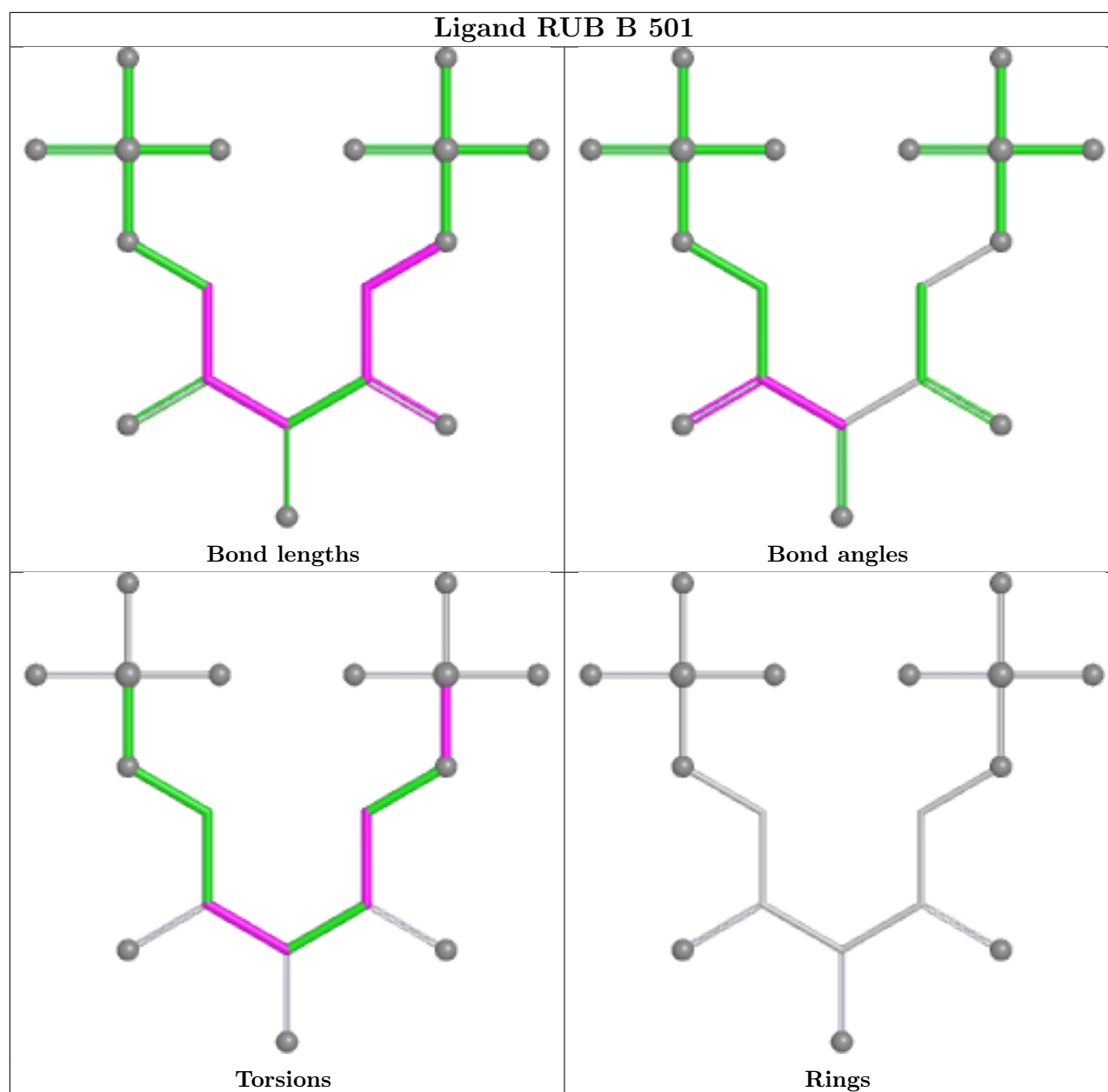
4 monomers are involved in 8 short contacts:

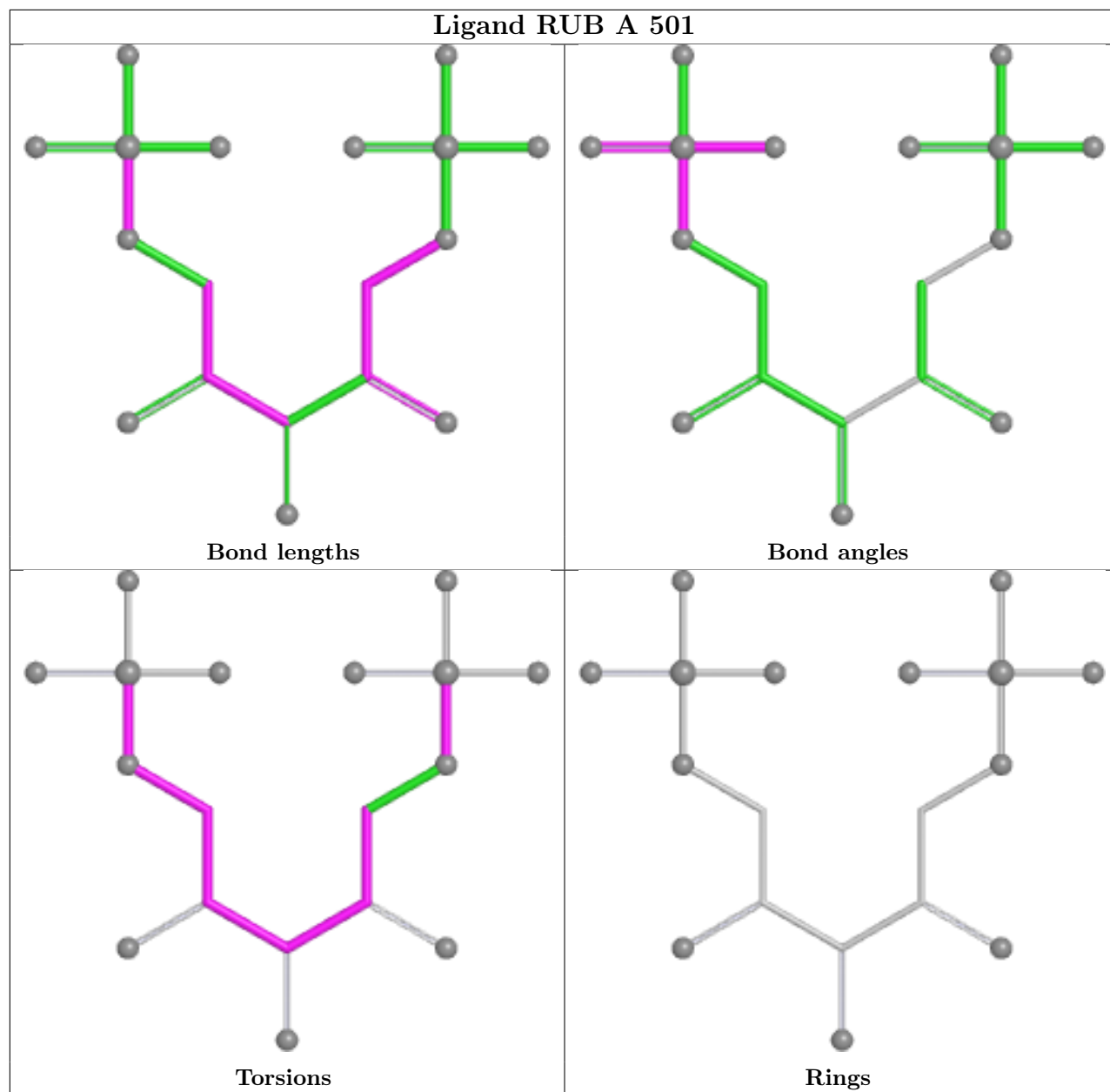
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	RUB	1	0
3	D	501	RUB	1	0
3	A	501	RUB	1	0
5	B	502	A8S	5	0

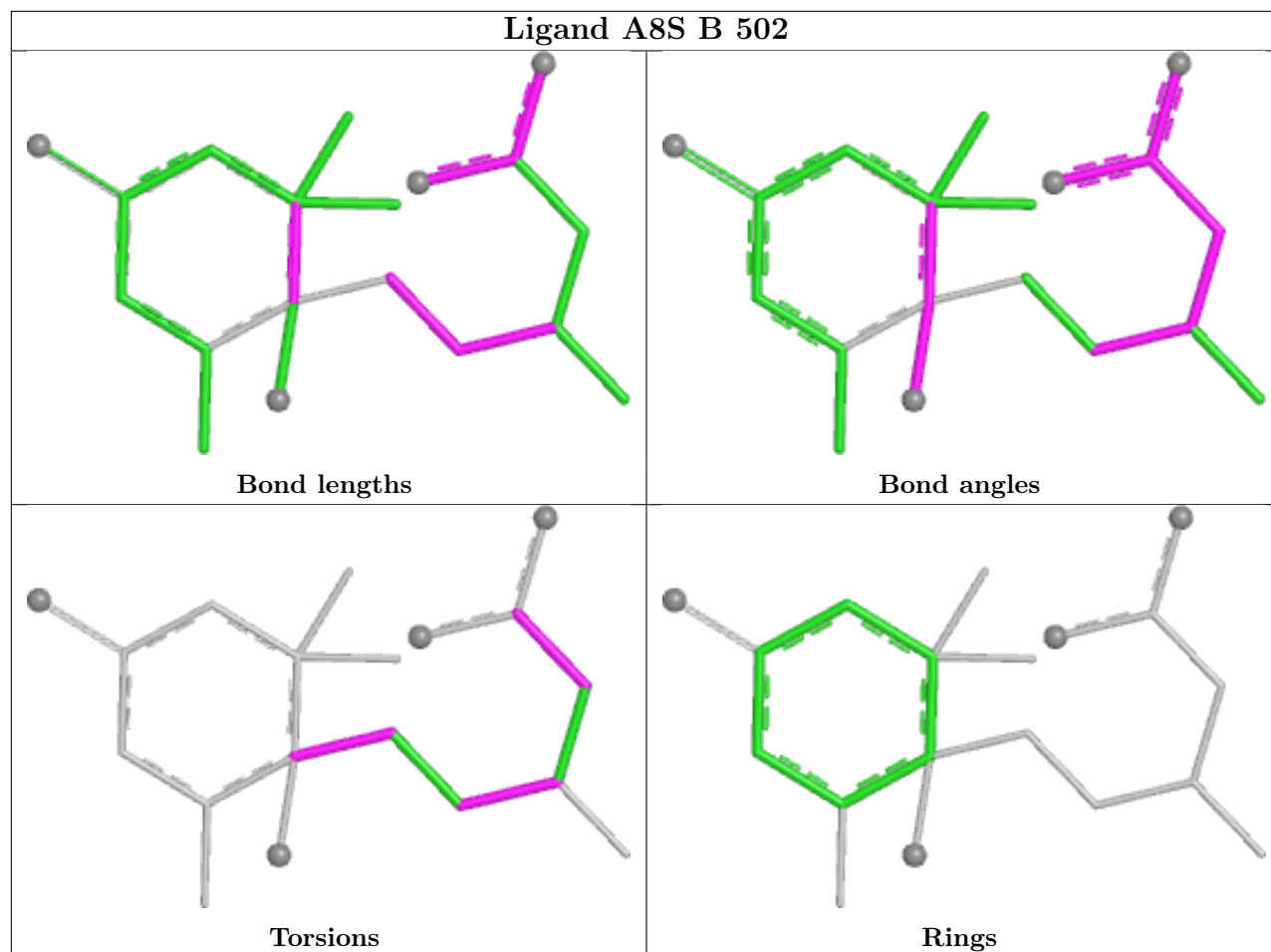
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	458/458 (100%)	-0.34	6 (1%) 75 78	8, 22, 46, 79	3 (0%)
1	B	458/458 (100%)	-0.33	9 (1%) 65 69	11, 23, 48, 87	4 (0%)
1	C	458/458 (100%)	-0.04	10 (2%) 62 66	14, 28, 54, 85	5 (1%)
1	D	458/458 (100%)	-0.08	9 (1%) 65 69	9, 27, 52, 88	5 (1%)
2	S	123/123 (100%)	0.00	2 (1%) 70 74	17, 28, 52, 65	0
2	T	123/123 (100%)	-0.03	2 (1%) 70 74	15, 30, 53, 58	1 (0%)
2	U	123/123 (100%)	0.52	7 (5%) 29 33	19, 37, 63, 78	2 (1%)
2	V	123/123 (100%)	0.34	7 (5%) 29 33	20, 34, 58, 68	0
All	All	2324/2324 (100%)	-0.11	52 (2%) 62 66	8, 27, 53, 88	20 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	465	ILE	5.1
1	D	469	PHE	4.7
2	U	77	THR	4.5
1	B	469	PHE	4.0
1	C	465	ILE	3.9
1	B	91	PRO	3.8
1	D	467	PHE	3.3
1	A	469	PHE	3.3
1	C	469	PHE	3.2
2	V	92	LYS	3.1
1	C	467	PHE	3.1
1	D	462[A]	TRP	3.0
1	C	92	GLY	3.0
2	S	121	ALA	3.0
2	U	110	VAL	2.7
1	D	94	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	12	GLY	2.6
2	V	121	ALA	2.6
2	T	92	LYS	2.6
2	V	77	THR	2.5
2	S	123	TYR	2.5
1	D	95	ASN	2.5
1	A	451	TRP	2.5
1	B	92	GLY	2.5
2	V	91	LYS	2.5
2	U	23	ARG	2.5
1	B	90	VAL	2.4
1	A	465	ILE	2.4
1	B	465	ILE	2.4
1	A	93	GLU	2.3
2	V	90	VAL	2.3
1	C	127	PHE	2.3
1	C	463	LYS	2.3
2	T	122	GLY	2.3
1	C	14	LYS	2.2
2	U	85	LYS	2.2
1	B	445	ILE	2.2
1	A	12	GLY	2.2
1	D	93	GLU	2.2
1	C	451	TRP	2.2
1	B	467	PHE	2.1
2	V	85	LYS	2.1
1	B	127	PHE	2.1
1	A	338	GLU	2.1
1	D	466	LYS	2.1
1	D	451	TRP	2.1
1	C	464	GLU	2.0
2	U	121	ALA	2.1
2	U	122	GLY	2.0
2	V	122	GLY	2.0
1	B	94	ASP	2.0
2	U	91	LYS	2.0

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

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](#)

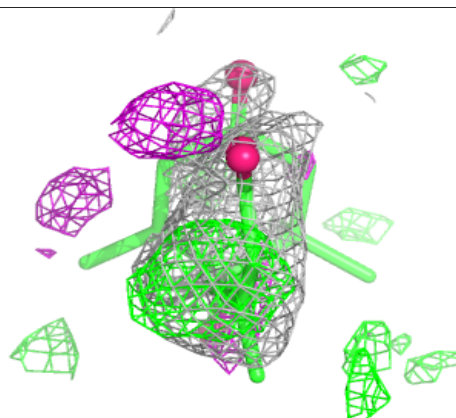
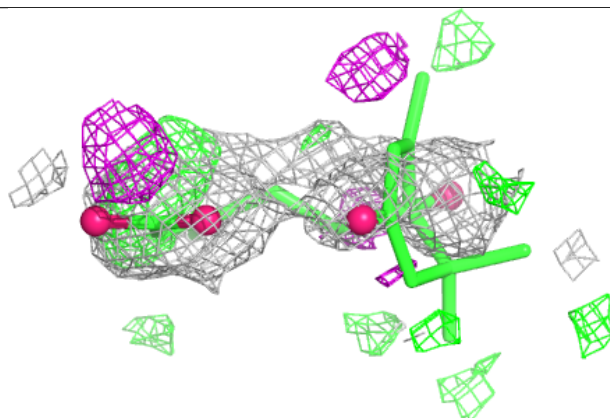
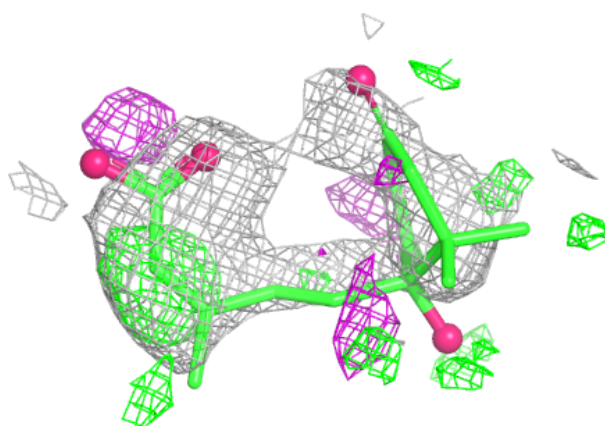
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	A8S	B	502	19/19	0.71	0.35	96,102,104,104	0
4	PO4	C	502	5/5	0.90	0.11	70,70,71,71	0
4	PO4	A	502	5/5	0.90	0.14	70,73,75,75	0
4	PO4	D	502	5/5	0.91	0.12	65,65,66,67	0
3	RUB	D	501	18/18	0.92	0.11	34,45,57,60	0
3	RUB	A	501	18/18	0.95	0.09	22,35,46,50	0
3	RUB	C	501	18/18	0.96	0.07	36,41,49,49	0
3	RUB	B	501	18/18	0.96	0.08	25,35,45,47	0

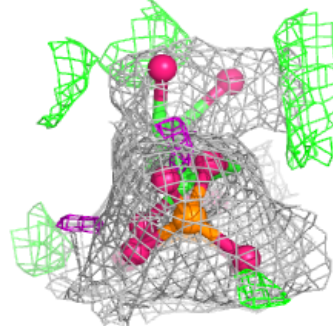
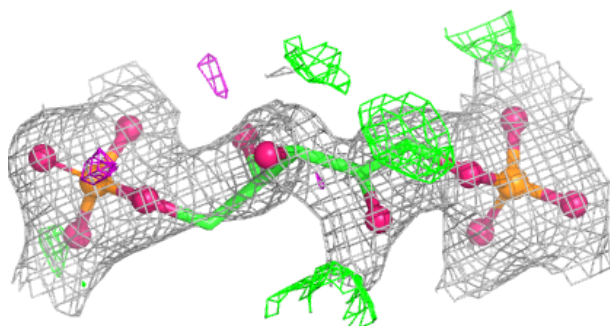
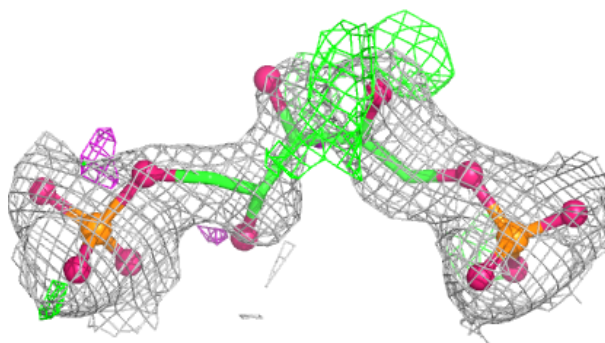
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A8S B 502:

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

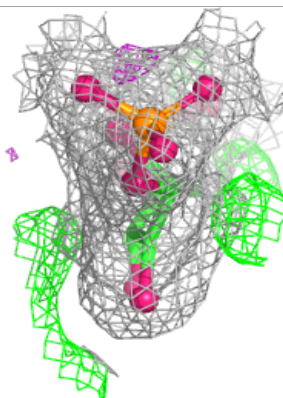
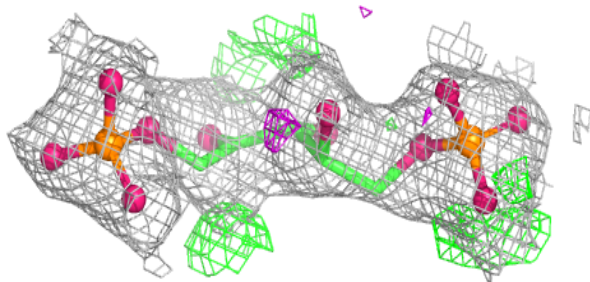
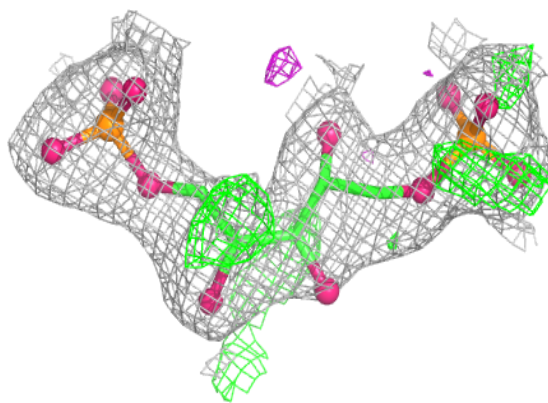
**Electron density around RUB D 501:**

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

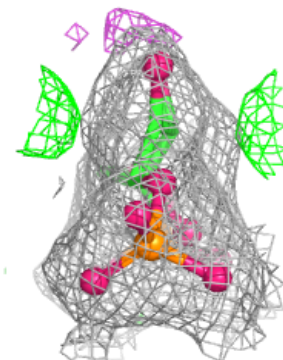
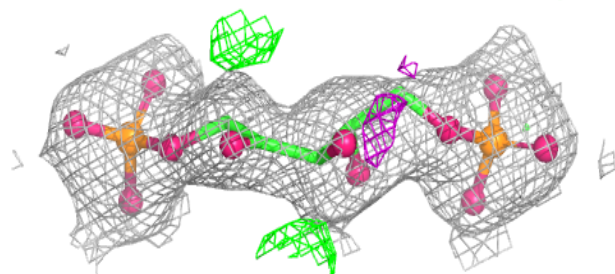
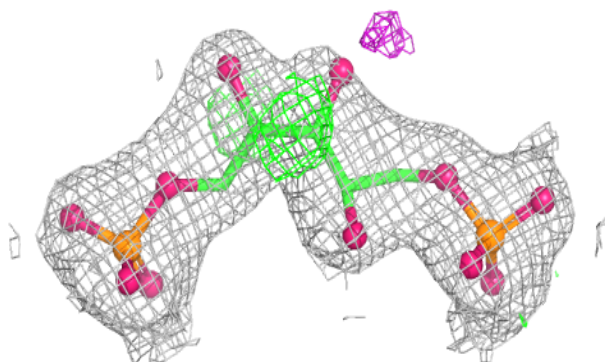


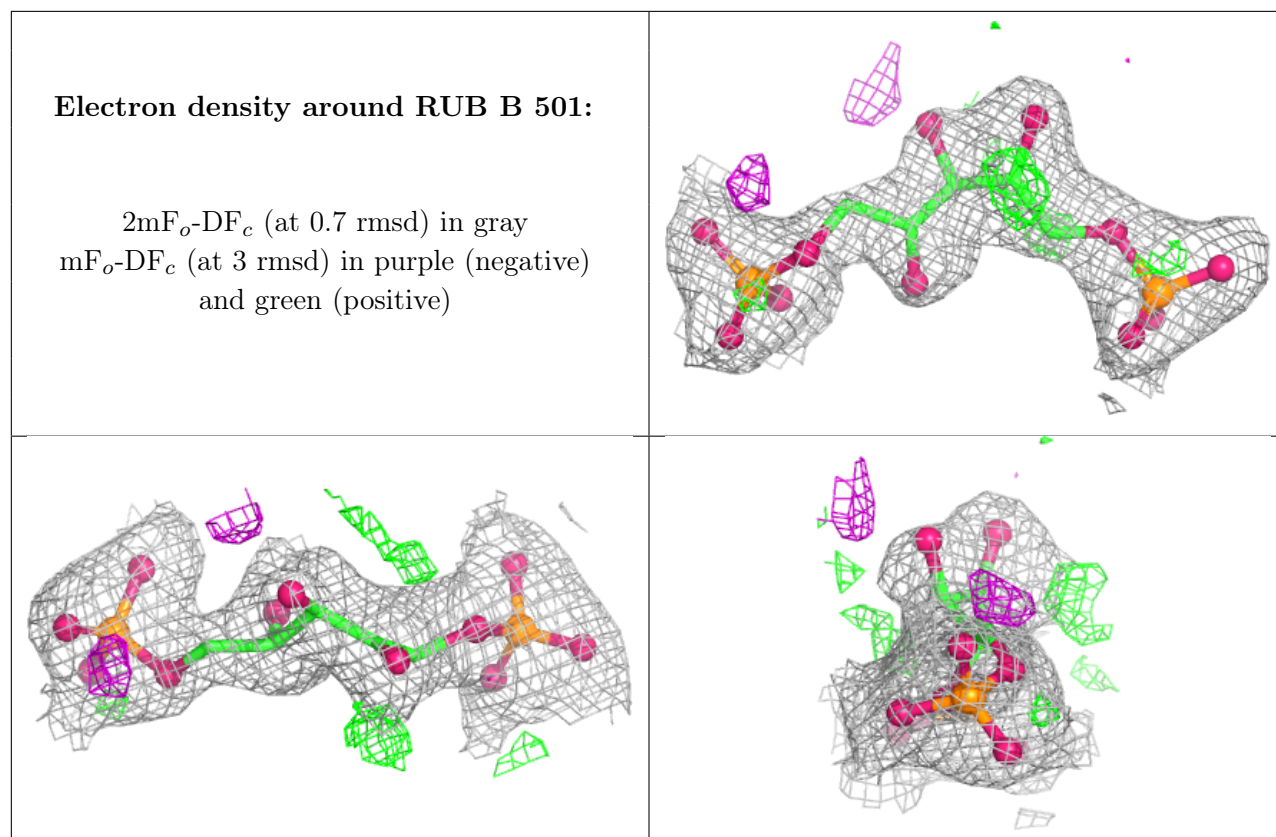
Electron density around RUB A 501:

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

**Electron density around RUB C 501:**

$2mF_o-DF_c$ (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.