wwPDB X-ray Structure Validation Summary Report (i)

Jun 29, 2024 – 01:25 AM EDT

PDB ID	:	9RUB
Title	:	CRYSTAL STRUCTURE OF ACTIVATED RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE COMPLEXED WITH ITS SUBSTRATE, RIBULOSE-1,5-BISPHOSPHATE
Authors	:	Lundqvist, T.; Schneider, G.
Deposited on	:	1990-11-28
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

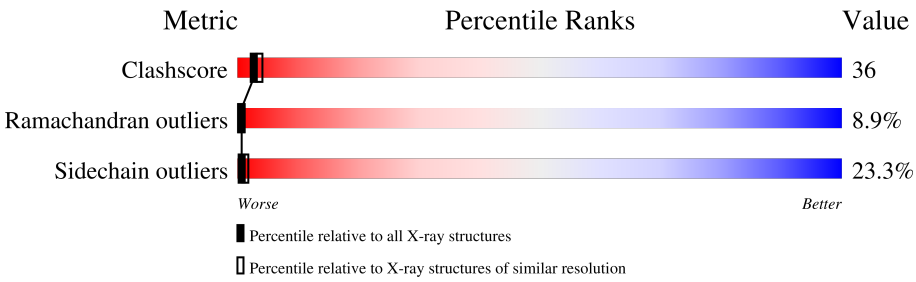
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	466	19% 44% 24% 12% •
1	B	466	29% 35% 27% 8% •

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	FMT	A	601	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7044 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.

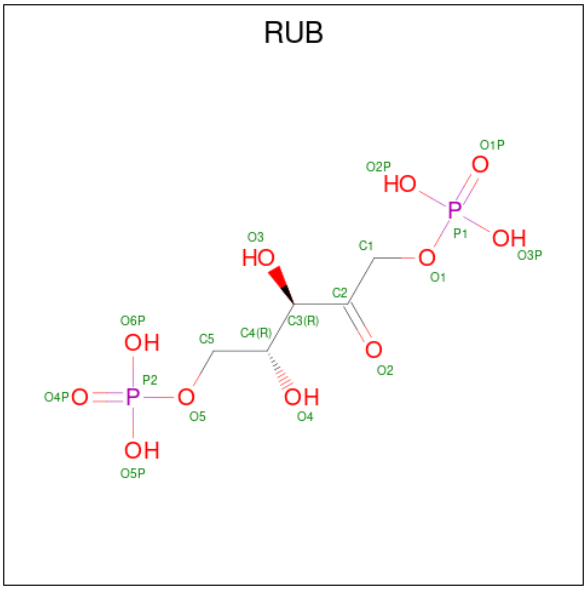
- Molecule 1 is a protein called RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	459	3502	2213	613	658	18	8	0	0
1	B	458	3498	2211	612	657	18	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASP	HIS	conflict	UNP P04718
B	91	ASP	HIS	conflict	UNP P04718

- Molecule 2 is RIBULOSE-1,5-DIPHOSPHATE (three-letter code: RUB) (formula: $C_5H_{12}O_{11}P_2$).



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

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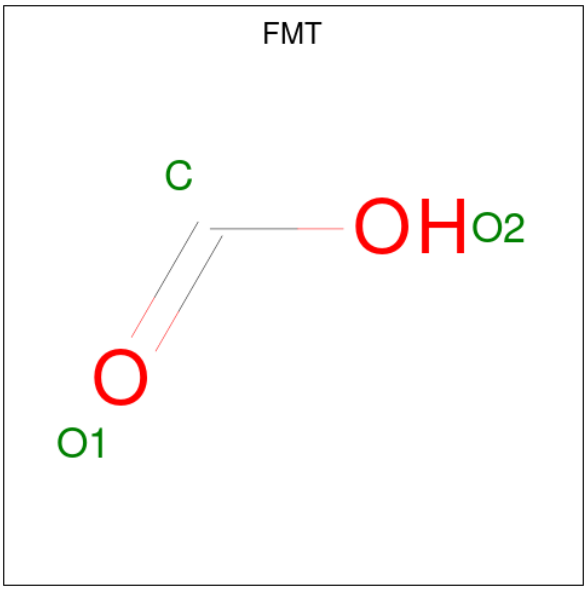
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	B	1	18	5	11	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
			Total	Mg		
3	B	1	1	1	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	3	1	2		0	0
			Total	C	O			
4	B	1	3	1	2		0	0

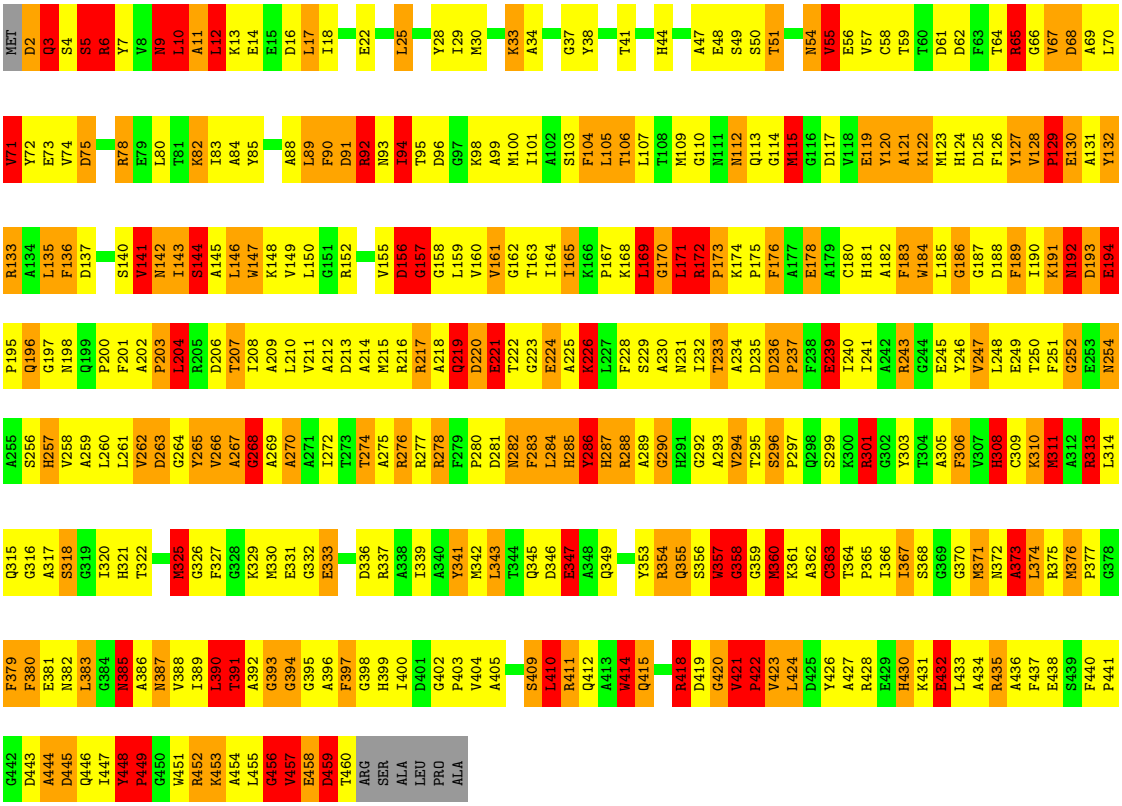
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

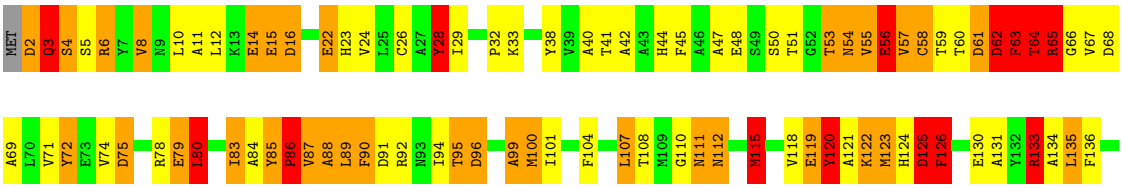
• Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE

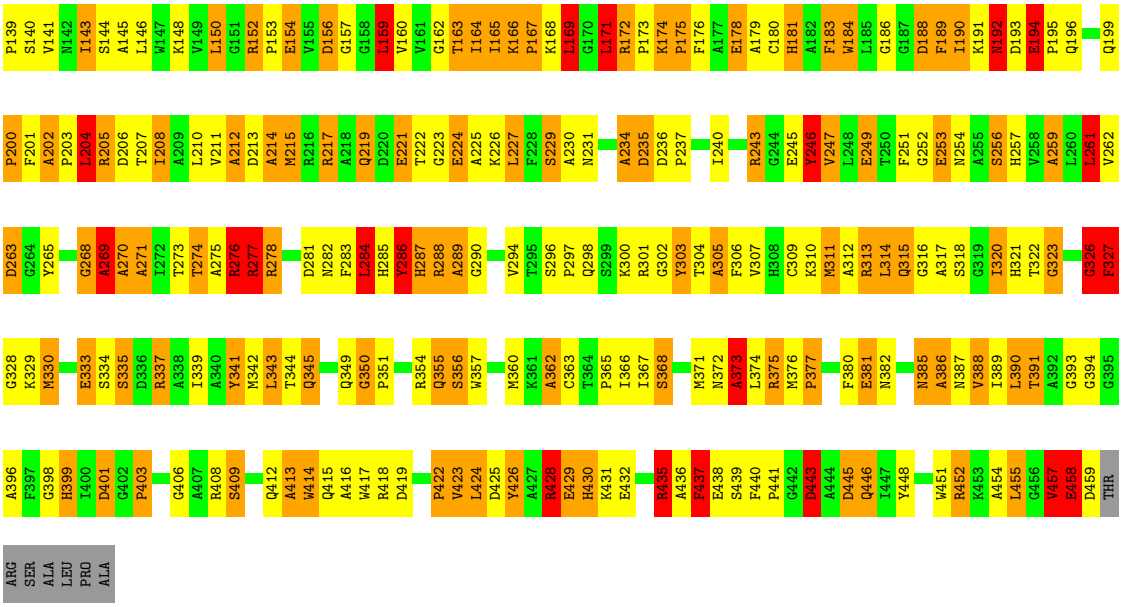
Chain A: 19% 44% 24% 12% •



• Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE

Chain B: 29% 35% 27% 8% •




P139 S140 V141 N142 I143 S144 A145 L146 W147 K148 V149 L150 G151 R152 P153 E154 V155 D156 G157 G158 L159 V160 V161 G162 T163 I164 I165 K166 P167 K168 L169 G170 L171 R172 P173 K174 P175 F176 A177 E178 A179 C180 H181 A182 F183 W184 L185 G186 G187 D188 F189 I190 K191 N192 D193 E194 P195 Q196 Q199
P200 F201 A202 P203 L204 R205 D206 T207 I208 A209 L210 V211 A212 D213 A214 M215 R216 R217 A218 Q219 D220 E221 T222 G223 E224 A225 K226 L227 F228 S229 A230 N231 A234 D235 D236 P237 I240 R243 G244 E245 Y246 V247 L248 E249 T250 F251 G252 E253 N254 A255 S256 H257 V258 A259 L260 L261 V262
D263 G264 Y265 G268 A269 A270 A271 I272 T273 T274 A275 R276 R277 R278 D281 N282 F283 L284 H285 Y286 H287 R288 A289 G290 V294 T295 S296 P297 Q298 S299 K300 R301 G302 Y303 T304 A305 F306 V307 H308 C309 K310 M311 A312 R313 L314 Q315 G316 A317 S318 G319 I320 H321 T322 G323 G326 F327
G328 K329 M330 E333 S334 S335 D336 R337 A338 I339 A340 Y341 M342 L343 T344 Q345 Q349 G350 P351 R354 Q355 S356 W357 M360 K361 A362 C363 T364 P365 I366 I367 S368 M371 N372 A373 L374 R375 M376 P377 F380 E381 N382 N385 A386 N387 V388 I389 L390 T391 A392 G393 G394 G395
A396 F397 G398 H399 I400 D401 G402 P403 G406 A407 R408 S409 Q412 A413 W414 Q415 A416 W417 R418 D419 P422 V423 L424 D425 Y426 A427 R428 E429 H430 K431 E432 R435 A436 F437 E438 S439 F440 P441 G442 D443 A444 D445 Q446 I447 Y448 W451 R452 K453 A454 L455 G456 V457 E458 D459 THR
ARG SER ALA LEU PRO ALA

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.50Å 70.60Å 104.10Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7044	wwPDB-VP
Average B, all atoms ($Å^2$)	19.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, MG, 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	1.14	4/3586 (0.1%)	2.90	360/4859 (7.4%)
1	B	1.02	1/3582 (0.0%)	2.84	300/4854 (6.2%)
All	All	1.08	5/7168 (0.1%)	2.87	660/9713 (6.8%)

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	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	458	GLU	CG-CD	21.57	1.84	1.51
1	A	459	ASP	CG-OD2	13.53	1.56	1.25
1	A	460	THR	N-CA	-10.23	1.25	1.46
1	B	457	VAL	C-O	-9.22	1.05	1.23
1	A	459	ASP	CB-CG	-5.24	1.40	1.51

The worst 5 of 660 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	428	ARG	CD-NE-CZ	38.62	177.67	123.60
1	B	65	ARG	CD-NE-CZ	26.96	161.35	123.60
1	A	78	ARG	CD-NE-CZ	23.14	156.00	123.60
1	A	96	ASP	CB-CG-OD1	20.82	137.03	118.30
1	A	459	ASP	C-N-CA	20.41	172.74	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	457	VAL	Mainchain

5.2 Too-close contacts (i)

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	3502	0	3368	276	0
1	B	3498	0	3371	244	0
2	A	18	0	8	3	0
2	B	18	0	7	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	3	0	0	2	0
4	B	3	0	0	1	0
All	All	7044	0	6754	496	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 36.

The worst 5 of 496 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:234:ALA:HB3	1:B:240:ILE:HG13	1.25	1.11
1:B:321:HIS:HB3	2:B:700:RUB:O6P	1.56	1.05
1:A:167:PRO:HD3	1:B:59:THR:HG21	1.41	1.01
1:A:285:HIS:HE2	1:A:321:HIS:HE2	1.05	0.94
1:B:322:THR:HG22	1:B:323:GLY:H	1.34	0.92

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	457/466 (98%)	330 (72%)	82 (18%)	45 (10%)	0 0
1	B	456/466 (98%)	360 (79%)	60 (13%)	36 (8%)	1 1
All	All	913/932 (98%)	690 (76%)	142 (16%)	81 (9%)	1 0

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	38	TYR
1	A	129	PRO
1	A	136	PHE
1	A	144	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	348/354 (98%)	266 (76%)	82 (24%)	1 1
1	B	348/354 (98%)	268 (77%)	80 (23%)	1 1
All	All	696/708 (98%)	534 (77%)	162 (23%)	1 1

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	169	LEU

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Mol	Chain	Res	Type
1	B	377	PRO
1	B	180	CYS
1	B	249	GLU
1	B	424	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	181	HIS
1	B	382	ASN
1	B	415	GLN
1	B	385	ASN
1	B	315	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	RUB	B	700	3	15,17,17	1.55	2 (13%)	16,25,25	0.88	0
2	RUB	A	600	3	15,17,17	2.83	8 (53%)	16,25,25	1.49	4 (25%)
4	FMT	A	601	1,3	2,2,2	1.37	0	1,1,1	0.81	0
4	FMT	B	701	1,3	2,2,2	1.66	1 (50%)	1,1,1	1.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RUB	B	700	3	-	15/20/20/20	-
2	RUB	A	600	3	-	11/20/20/20	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	RUB	C5-C4	7.19	1.62	1.51
2	A	600	RUB	C1-C2	3.85	1.57	1.51
2	A	600	RUB	P2-O4P	3.33	1.61	1.50
2	A	600	RUB	P1-O1P	3.17	1.60	1.50
2	B	700	RUB	P1-O1P	3.17	1.60	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	RUB	O6P-P2-O5	2.48	113.34	106.73
2	A	600	RUB	O3P-P1-O1	2.28	112.79	106.73
2	A	600	RUB	O5-P2-O4P	2.26	112.82	106.47
2	A	600	RUB	O5-C5-C4	2.09	114.93	109.36

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	RUB	O2-C2-C3-O3
2	A	600	RUB	C2-C3-C4-C5
2	A	600	RUB	C2-C3-C4-O4
2	A	600	RUB	O3-C3-C4-C5
2	A	600	RUB	O3-C3-C4-O4

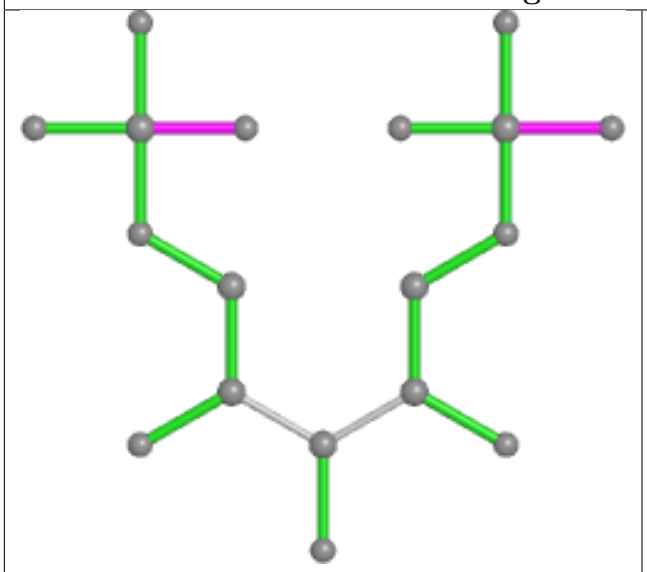
There are no ring outliers.

4 monomers are involved in 10 short contacts:

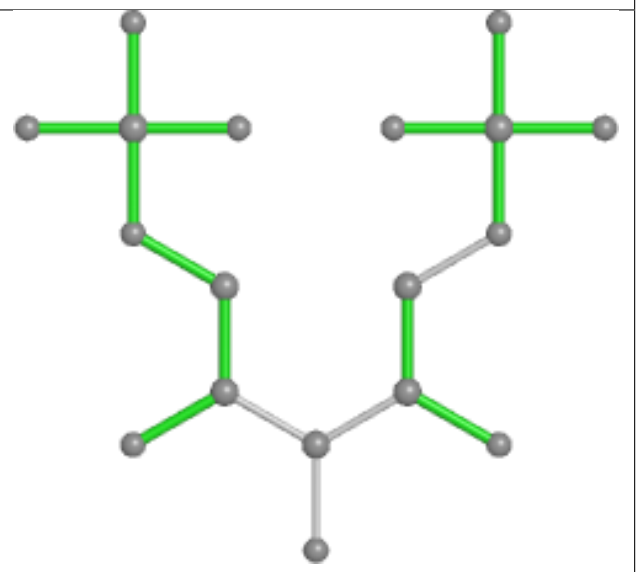
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	700	RUB	5	0
2	A	600	RUB	3	0
4	A	601	FMT	2	0
4	B	701	FMT	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

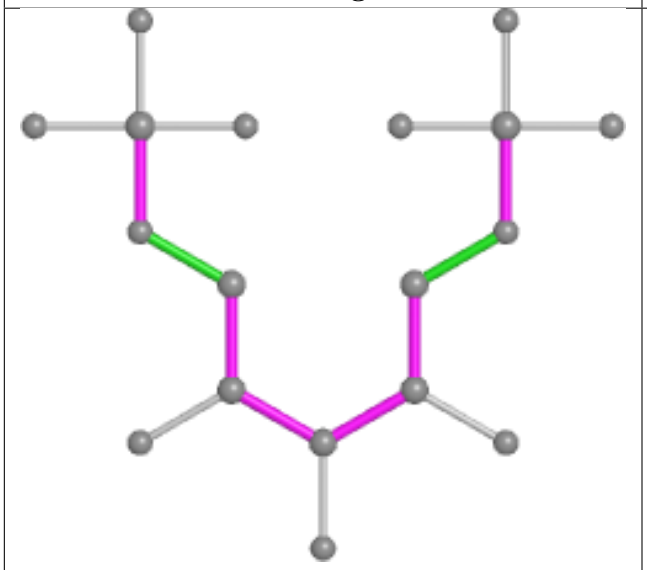
Ligand RUB B 700



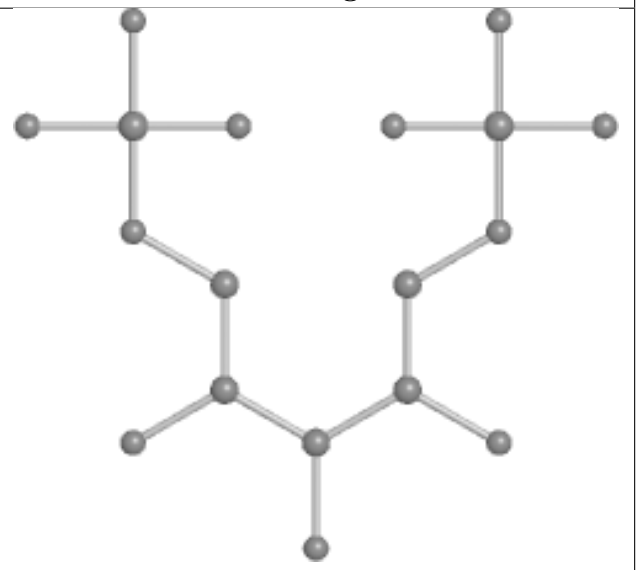
Bond lengths



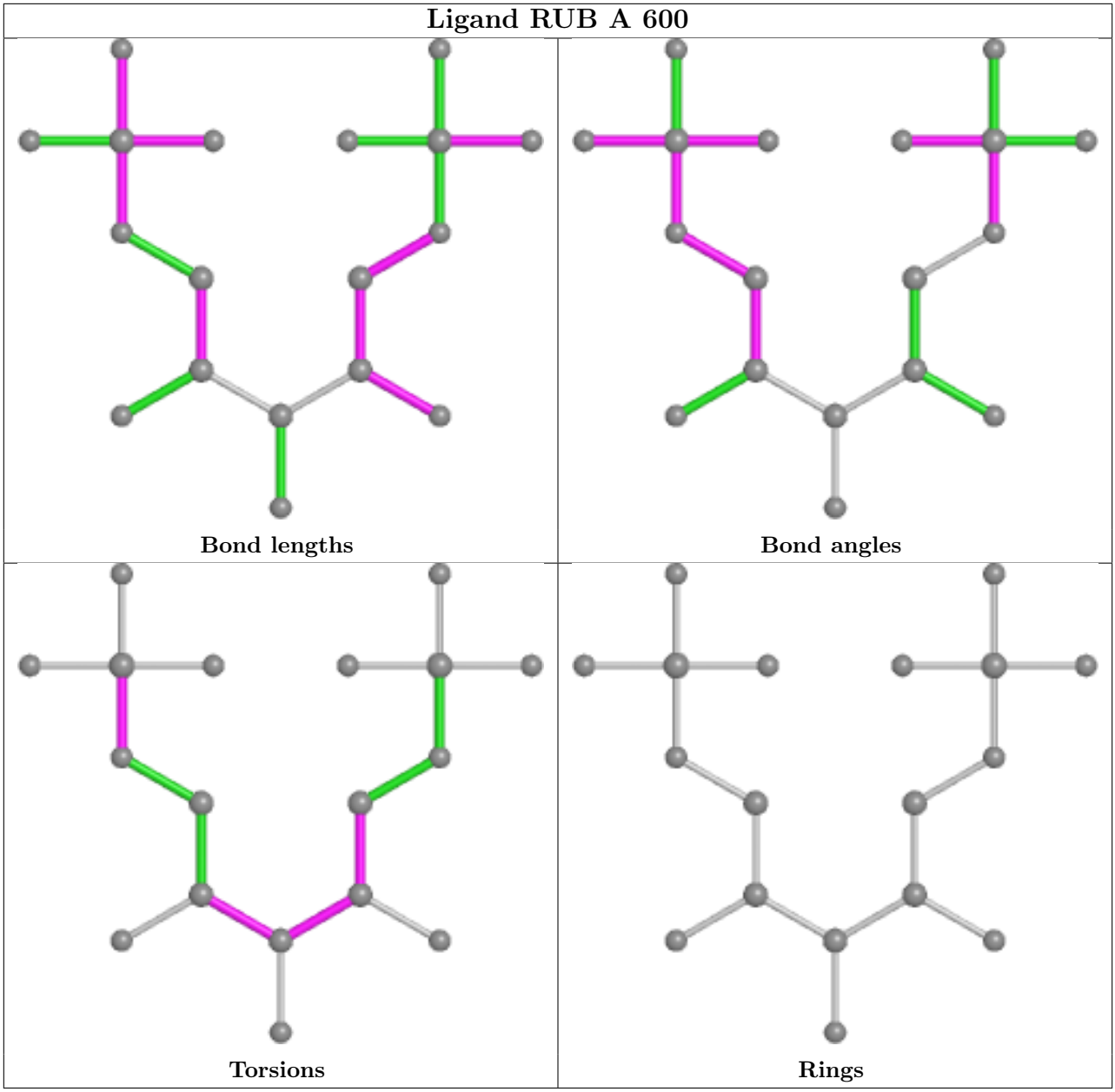
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.