



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2025 – 02:39 PM JST

PDB ID : 9W96 / pdb_00009w96
Title : Crystal structure of BioZ C115S from Agrobacterium tumefaciens in complex with galutaryl-CoA
Authors : Zhang, L.; Zhang, L.
Deposited on : 2025-08-09
Resolution : 2.50 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

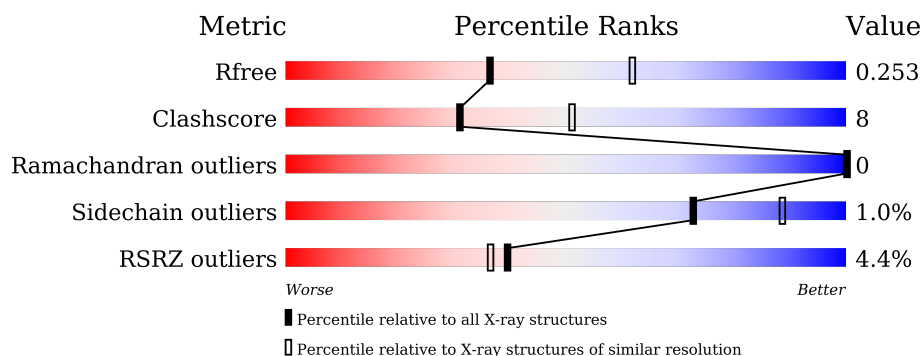
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	327	
1	B	327	
1	C	327	
1	D	327	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9931 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.

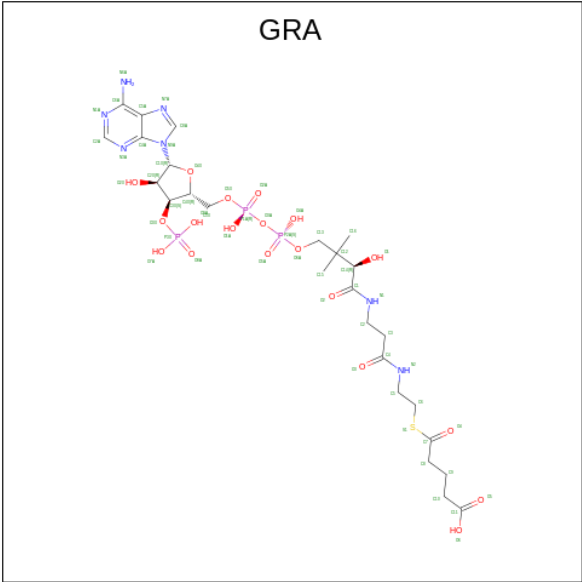
- Molecule 1 is a protein called 3-oxopimeloyl-[acyl-carrier-protein] synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2374	1471	435	457	11			
1	B	327	Total	C	N	O	S	0	0	0
			2383	1476	437	459	11			
1	C	327	Total	C	N	O	S	0	0	0
			2383	1476	437	459	11			
1	D	327	Total	C	N	O	S	0	0	0
			2383	1476	437	459	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	SER	CYS	engineered mutation	UNP Q7CTU0
B	115	SER	CYS	engineered mutation	UNP Q7CTU0
C	115	SER	CYS	engineered mutation	UNP Q7CTU0
D	115	SER	CYS	engineered mutation	UNP Q7CTU0

- Molecule 2 is glutaryl-coenzyme A (CCD ID: GRA) (formula: C₂₆H₄₂N₇O₁₉P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		

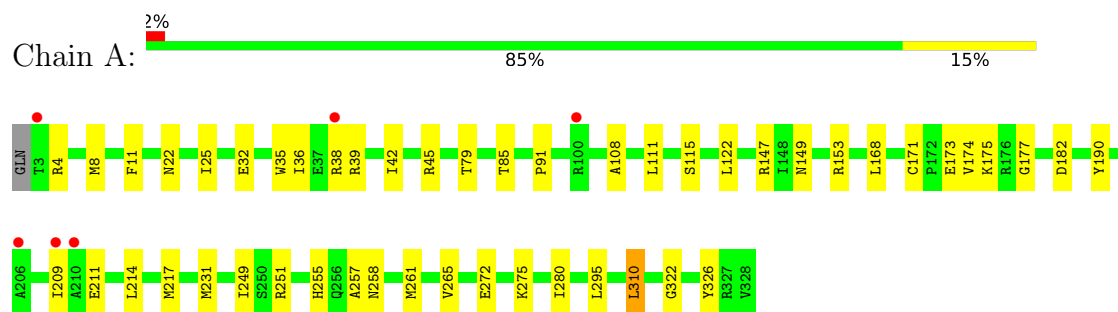
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	58	Total	O	0	0
			58	58		
3	C	50	Total	O	0	0
			50	50		
3	D	18	Total	O	0	0
			18	18		

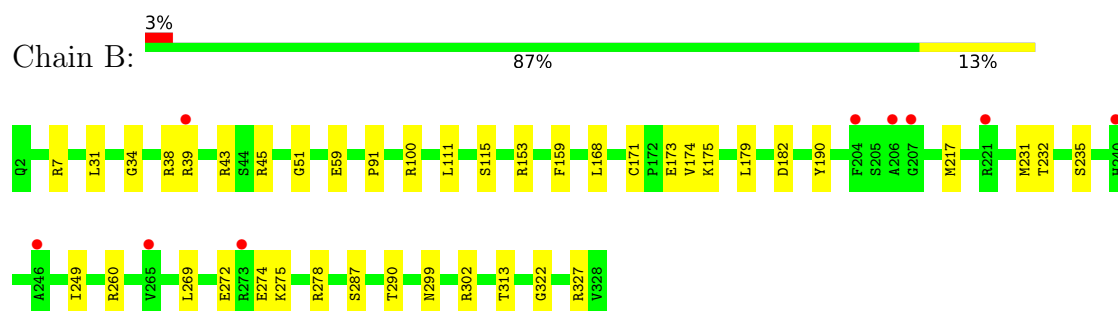
3 Residue-property plots [i](#)

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.

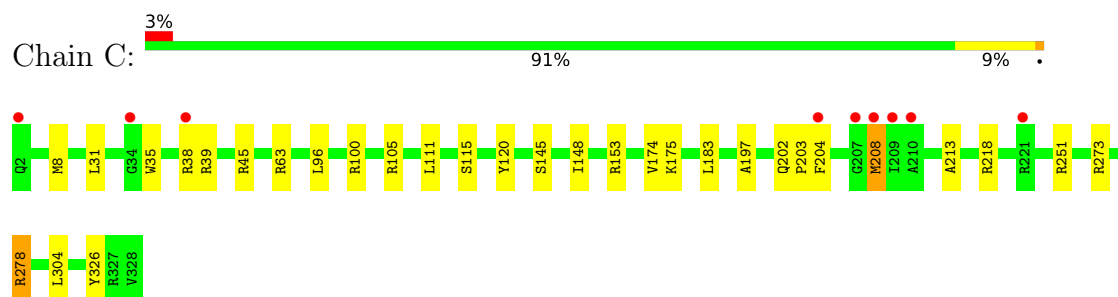
- Molecule 1: 3-oxopimeloyl-[acyl-carrier-protein] synthase



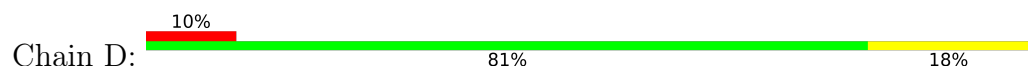
- Molecule 1: 3-oxopimeloyl-[acyl-carrier-protein] synthase

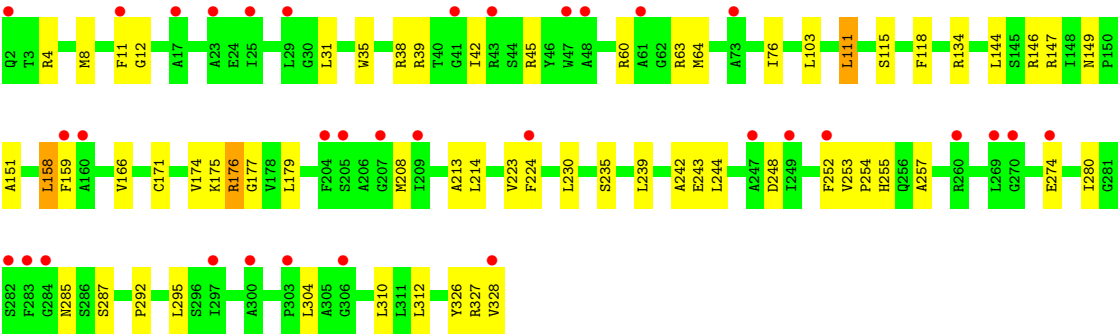


- Molecule 1: 3-oxopimeloyl-[acyl-carrier-protein] synthase



- Molecule 1: 3-oxopimeloyl-[acyl-carrier-protein] synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.72Å 128.45Å 170.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.05 – 2.50 47.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.2 (47.05-2.50) 90.6 (47.05-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.51Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, R_{free}	0.216 , 0.254 0.217 , 0.253	Depositor DCC
R_{free} test set	2153 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9931	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/2407	0.83	0/3267
1	B	0.46	0/2416	0.84	0/3279
1	C	0.46	0/2416	0.84	0/3279
1	D	0.44	0/2416	0.86	0/3279
All	All	0.46	0/9655	0.84	0/13104

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2374	0	2393	46	0
1	B	2383	0	2401	31	0
1	C	2383	0	2401	32	0
1	D	2383	0	2401	55	0
2	A	56	0	37	6	0
2	B	56	0	37	4	0
2	C	56	0	37	3	0
2	D	56	0	37	4	0
3	A	58	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	58	0	0	0	0
3	C	50	0	0	0	0
3	D	18	0	0	0	0
All	All	9931	0	9744	158	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 (158) 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:8:MET:HE1	1:D:295:LEU:HD13	1.53	0.87
1:D:42:ILE:HD11	1:D:158:LEU:HD23	1.61	0.82
1:C:31:LEU:HD21	1:C:153:ARG:HD2	1.63	0.79
1:C:218:ARG:HH11	1:C:218:ARG:HG3	1.48	0.78
1:A:8:MET:HE1	1:A:295:LEU:HD13	1.66	0.77
1:A:4:ARG:HG3	1:A:174:VAL:HG22	1.67	0.77
1:C:31:LEU:HD23	1:C:35:TRP:CD2	2.22	0.74
1:A:153:ARG:HH21	2:A:401:GRA:H5XA	1.54	0.72
1:C:208:MET:HE1	1:C:213:ALA:HB2	1.72	0.71
1:A:258:ASN:HD21	2:A:401:GRA:H13	1.58	0.69
1:B:231:MET:HE3	1:B:313:THR:HG23	1.75	0.68
1:A:258:ASN:ND2	2:A:401:GRA:H13	2.09	0.68
1:B:217:MET:SD	2:B:401:GRA:H3	2.34	0.67
1:A:38:ARG:HH21	1:A:39:ARG:HD2	1.60	0.67
1:A:209:ILE:HG22	1:A:211:GLU:HB3	1.77	0.66
1:B:43:ARG:HH22	1:B:278:ARG:HH12	1.43	0.66
1:B:272:GLU:HB3	1:B:274:GLU:OE1	1.94	0.66
1:C:203:PRO:HG2	1:D:146:ARG:HD3	1.78	0.65
1:A:35:TRP:O	1:A:38:ARG:HG2	1.96	0.65
1:D:158:LEU:HD21	1:D:257:ALA:O	1.96	0.65
1:C:278:ARG:HH11	1:C:278:ARG:HB2	1.62	0.64
1:D:76:ILE:HG21	1:D:103:LEU:HD13	1.78	0.63
1:D:42:ILE:HG12	1:D:280:ILE:HG12	1.79	0.63
1:D:134:ARG:HH11	1:D:134:ARG:HG3	1.62	0.63
1:D:4:ARG:HG2	1:D:174:VAL:HG22	1.81	0.61
1:D:12:GLY:HA2	1:D:64:MET:HE2	1.82	0.61
1:A:257:ALA:HB1	2:A:401:GRA:H5	1.81	0.61
1:D:176:ARG:HH12	1:D:328:VAL:C	2.09	0.60
1:A:8:MET:HE2	1:A:11:PHE:CE2	2.37	0.59
1:A:272:GLU:OE2	1:A:275:LYS:HD3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LEU:HG	1:C:100:ARG:HD2	1.83	0.59
1:D:235:SER:O	1:D:239:LEU:HD22	2.04	0.58
1:A:251:ARG:HB2	1:A:310:LEU:HD22	1.85	0.57
1:B:115:SER:OG	2:B:401:GRA:C7	2.52	0.57
1:D:177:GLY:HA2	1:D:326:TYR:HE1	1.69	0.57
1:C:278:ARG:HB2	1:C:278:ARG:NH1	2.20	0.57
1:D:149:ASN:C	1:D:149:ASN:HD22	2.12	0.56
1:A:42:ILE:HG12	1:A:280:ILE:HG12	1.88	0.55
1:B:34:GLY:O	1:B:38:ARG:HG2	2.06	0.55
1:A:38:ARG:HG3	1:A:39:ARG:HG3	1.89	0.55
1:D:255:HIS:CD2	1:D:257:ALA:HB2	2.41	0.55
1:C:218:ARG:HG3	1:C:218:ARG:NH1	2.19	0.54
1:B:174:VAL:HG12	1:B:175:LYS:H	1.73	0.54
1:C:31:LEU:HD23	1:C:35:TRP:CE2	2.43	0.54
1:C:208:MET:O	1:C:208:MET:HG3	2.07	0.53
1:D:134:ARG:HG3	1:D:134:ARG:NH1	2.23	0.53
1:D:179:LEU:HD11	1:D:327:ARG:HB2	1.91	0.53
1:C:278:ARG:HH11	1:C:278:ARG:CB	2.22	0.52
1:D:177:GLY:HA2	1:D:326:TYR:CE1	2.44	0.52
1:D:118:PHE:CE2	1:D:292:PRO:HB3	2.45	0.52
1:A:182:ASP:O	1:A:322:GLY:HA2	2.10	0.52
1:C:115:SER:OG	2:C:401:GRA:C7	2.57	0.52
1:D:147:ARG:HA	1:D:214:LEU:HD12	1.90	0.52
1:C:204:PHE:HE1	1:C:208:MET:HE2	1.74	0.52
1:A:255:HIS:CD2	1:A:257:ALA:HB2	2.45	0.52
1:A:174:VAL:HG12	1:A:175:LYS:N	2.26	0.51
1:C:197:ALA:HB2	1:C:202:GLN:OE1	2.10	0.51
1:C:174:VAL:HG12	1:C:175:LYS:N	2.26	0.51
1:D:8:MET:HE2	1:D:11:PHE:CE1	2.46	0.51
1:C:8:MET:HG3	1:C:326:TYR:CZ	2.45	0.51
1:B:174:VAL:HG12	1:B:175:LYS:N	2.26	0.51
1:B:51:GLY:HA2	1:C:63:ARG:HG2	1.93	0.51
1:B:179:LEU:HD11	1:B:327:ARG:HB2	1.93	0.51
1:A:174:VAL:HG12	1:A:175:LYS:H	1.76	0.50
1:D:115:SER:OG	1:D:287:SER:HA	2.11	0.50
1:D:242:ALA:O	1:D:244:LEU:HD12	2.12	0.50
1:C:45:ARG:HG2	1:C:45:ARG:HH11	1.77	0.49
1:A:190:TYR:CD1	1:B:91:PRO:HG2	2.47	0.49
1:B:51:GLY:HA2	1:C:63:ARG:CG	2.43	0.49
1:C:120:TYR:CD2	1:C:183:LEU:HD13	2.48	0.49
1:A:122:LEU:HD12	1:A:168:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:CD	1:A:275:LYS:HD3	2.38	0.48
1:A:4:ARG:HG3	1:A:174:VAL:CG2	2.42	0.48
1:B:39:ARG:HH22	2:B:401:GRA:C4X	2.26	0.48
1:B:327:ARG:HH11	1:B:327:ARG:HG2	1.79	0.48
1:A:32:GLU:O	1:A:35:TRP:HB2	2.14	0.48
1:C:38:ARG:NH2	1:C:39:ARG:HH12	2.12	0.47
1:D:174:VAL:HG12	1:D:175:LYS:H	1.79	0.47
1:A:149:ASN:HA	1:A:214:LEU:HD13	1.96	0.47
1:D:149:ASN:ND2	1:D:151:ALA:H	2.12	0.47
1:D:252:PHE:CE2	1:D:254:PRO:HG3	2.49	0.47
1:A:35:TRP:HA	1:A:38:ARG:HD3	1.97	0.47
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.79	0.47
1:A:115:SER:OG	2:A:401:GRA:C7	2.63	0.47
1:D:8:MET:HE3	1:D:166:VAL:HG21	1.96	0.47
1:A:231:MET:HE3	1:A:265:VAL:HG21	1.97	0.47
1:D:149:ASN:HD22	1:D:151:ALA:H	1.62	0.46
2:C:401:GRA:H2B	2:C:401:GRA:H14	1.78	0.46
1:D:304:LEU:HB3	1:D:328:VAL:HG21	1.96	0.46
1:A:111:LEU:HD22	1:B:111:LEU:HG	1.96	0.46
1:B:231:MET:CE	1:B:313:THR:HG23	2.44	0.46
1:A:249:ILE:O	1:A:275:LYS:HE3	2.15	0.46
1:C:38:ARG:HH21	1:C:39:ARG:HH12	1.63	0.46
1:A:91:PRO:HG2	1:B:190:TYR:CD1	2.51	0.46
1:A:171:CYS:SG	1:A:173:GLU:HG2	2.55	0.46
1:D:310:LEU:HD12	1:D:326:TYR:HD2	1.81	0.46
1:D:158:LEU:HD22	1:D:285:ASN:HB2	1.97	0.45
1:D:176:ARG:CZ	1:D:176:ARG:HB2	2.46	0.45
2:C:401:GRA:H15B	2:C:401:GRA:O2A	2.16	0.45
1:D:176:ARG:HB2	1:D:176:ARG:NH1	2.32	0.45
1:B:59:GLU:OE1	1:B:100:ARG:HD3	2.17	0.45
1:C:251:ARG:CZ	1:C:304:LEU:HD23	2.46	0.45
1:B:232:THR:HA	1:B:269:LEU:HD11	1.99	0.45
1:C:31:LEU:HD23	1:C:35:TRP:CG	2.52	0.45
1:A:39:ARG:NH1	2:A:401:GRA:H5X	2.32	0.45
1:B:171:CYS:SG	1:B:173:GLU:HG3	2.56	0.45
1:B:45:ARG:HG2	1:B:45:ARG:HH11	1.82	0.45
1:D:31:LEU:HD23	1:D:35:TRP:CG	2.52	0.44
1:C:120:TYR:CZ	1:C:183:LEU:HB3	2.52	0.44
1:D:64:MET:HE2	1:D:64:MET:HB3	1.74	0.44
1:B:287:SER:O	1:B:290:THR:HG23	2.18	0.44
1:C:38:ARG:HE	1:C:39:ARG:NH1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ARG:HH11	1:C:105:ARG:HD2	1.70	0.43
1:C:204:PHE:CD2	1:C:204:PHE:C	2.96	0.43
1:D:174:VAL:HG12	1:D:175:LYS:N	2.34	0.43
1:D:224:PHE:HD2	2:D:401:GRA:H16B	1.83	0.43
1:D:244:LEU:HD23	1:D:248:ASP:HB3	2.00	0.43
1:D:242:ALA:O	1:D:243:GLU:HB2	2.17	0.43
1:D:244:LEU:HD23	1:D:248:ASP:CB	2.49	0.43
1:D:253:VAL:HB	1:D:312:LEU:HD23	2.00	0.43
1:A:79:THR:O	1:A:108:ALA:HA	2.19	0.42
1:A:190:TYR:CE1	1:B:91:PRO:HG2	2.53	0.42
1:D:42:ILE:CD1	1:D:158:LEU:HD23	2.38	0.42
1:D:60:ARG:HA	1:D:63:ARG:NH1	2.34	0.42
1:A:91:PRO:HG2	1:B:190:TYR:CE1	2.54	0.42
1:A:209:ILE:C	1:A:211:GLU:H	2.28	0.42
1:B:115:SER:OG	1:B:287:SER:HA	2.19	0.42
1:C:145:SER:HA	1:C:148:ILE:HD12	2.01	0.42
1:D:45:ARG:HH11	1:D:45:ARG:HG2	1.83	0.42
1:D:158:LEU:CD2	1:D:257:ALA:O	2.63	0.42
1:A:38:ARG:HG3	1:A:39:ARG:CG	2.49	0.42
1:D:39:ARG:HB3	2:D:401:GRA:O5A	2.19	0.42
1:D:208:MET:HE1	1:D:213:ALA:HB2	2.02	0.42
1:D:253:VAL:HB	1:D:312:LEU:CD2	2.49	0.42
1:B:31:LEU:HD21	1:B:153:ARG:HD3	2.02	0.42
1:D:223:VAL:HG11	2:D:401:GRA:HN2	1.84	0.42
1:A:25:ILE:HD11	1:A:45:ARG:HD2	2.02	0.42
1:B:249:ILE:O	1:B:275:LYS:HD3	2.19	0.42
1:B:159:PHE:CE1	2:B:401:GRA:H8B	2.54	0.42
1:B:182:ASP:O	1:B:322:GLY:HA2	2.20	0.42
1:A:177:GLY:HA2	1:A:326:TYR:CE2	2.55	0.41
1:D:144:LEU:HD13	1:D:159:PHE:CD1	2.55	0.41
1:B:235:SER:CB	1:B:269:LEU:HD21	2.50	0.41
2:D:401:GRA:H2B	2:D:401:GRA:H14	1.61	0.41
1:A:177:GLY:O	1:A:326:TYR:HA	2.20	0.41
1:B:7:ARG:O	1:B:168:LEU:HA	2.20	0.41
1:C:38:ARG:HE	1:C:39:ARG:HH12	1.69	0.41
1:C:111:LEU:HD22	1:D:111:LEU:HG	2.03	0.41
1:D:31:LEU:HD23	1:D:35:TRP:CE2	2.56	0.41
1:D:274:GLU:OE1	1:D:274:GLU:N	2.53	0.41
1:A:217:MET:HB2	1:A:217:MET:HE3	1.66	0.40
1:A:231:MET:HE1	1:A:261:MET:SD	2.61	0.40
1:D:38:ARG:HH21	1:D:39:ARG:CZ	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:LEU:HD23	1:D:230:LEU:HA	1.95	0.40
1:A:85:THR:HG22	1:A:147:ARG:HD2	2.03	0.40
1:D:171:CYS:SG	1:D:176:ARG:HD3	2.61	0.40
1:A:209:ILE:CG2	1:A:211:GLU:HB3	2.49	0.40
1:A:22:ASN:ND2	1:A:36:ILE:HB	2.36	0.40

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	324/327 (99%)	314 (97%)	10 (3%)	0	100	100
1	B	325/327 (99%)	318 (98%)	7 (2%)	0	100	100
1	C	325/327 (99%)	315 (97%)	10 (3%)	0	100	100
1	D	325/327 (99%)	316 (97%)	9 (3%)	0	100	100
All	All	1299/1308 (99%)	1263 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	239/240 (100%)	238 (100%)	1 (0%)	89	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	240/240 (100%)	237 (99%)	3 (1%)	65	85
1	C	240/240 (100%)	237 (99%)	3 (1%)	65	85
1	D	240/240 (100%)	237 (99%)	3 (1%)	65	85
All	All	959/960 (100%)	949 (99%)	10 (1%)	73	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	LEU
1	B	260	ARG
1	B	299	ASN
1	B	302	ARG
1	C	208	MET
1	C	273	ARG
1	C	278	ARG
1	D	111	LEU
1	D	158	LEU
1	D	176	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2	GLN
1	B	236	GLN
1	D	149	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

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GRA	D	401	-	50,58,58	0.77	2 (4%)	62,85,85	2.04	9 (14%)
2	GRA	B	401	-	50,58,58	0.96	3 (6%)	62,85,85	2.02	14 (22%)
2	GRA	C	401	-	50,58,58	0.91	3 (6%)	62,85,85	1.77	9 (14%)
2	GRA	A	401	-	50,58,58	0.94	2 (4%)	62,85,85	1.89	10 (16%)

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	GRA	D	401	-	-	23/53/73/73	0/3/3/3
2	GRA	B	401	-	-	19/53/73/73	0/3/3/3
2	GRA	C	401	-	-	32/53/73/73	0/3/3/3
2	GRA	A	401	-	-	23/53/73/73	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GRA	C7-S1	3.88	1.85	1.76
2	A	401	GRA	C7-S1	3.56	1.84	1.76
2	C	401	GRA	C7-S1	3.55	1.84	1.76
2	A	401	GRA	P3X-O3X	2.71	1.64	1.59
2	D	401	GRA	C7-S1	2.44	1.82	1.76
2	B	401	GRA	P3X-O3X	2.38	1.63	1.59
2	B	401	GRA	O4-C7	2.20	1.24	1.21
2	C	401	GRA	O4-C7	2.17	1.24	1.21
2	C	401	GRA	P3X-O3X	2.17	1.63	1.59
2	D	401	GRA	P3X-O3X	2.15	1.63	1.59

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GRA	C6-S1-C7	9.34	130.94	101.87
2	D	401	GRA	C6-S1-C7	7.33	124.70	101.87
2	D	401	GRA	C5-N2-C4	6.86	135.57	122.84
2	C	401	GRA	O4-C7-C8	-6.84	115.91	123.99
2	A	401	GRA	O4-C7-C8	-6.48	116.34	123.99
2	D	401	GRA	O4-C7-C8	-6.19	116.68	123.99
2	A	401	GRA	C6-S1-C7	5.84	120.05	101.87
2	B	401	GRA	C9-C8-C7	4.99	123.40	112.33
2	A	401	GRA	C6-C5-N2	4.90	122.72	112.42
2	D	401	GRA	C2-C3-C4	4.80	120.36	112.36
2	C	401	GRA	O4-C7-S1	4.77	128.81	122.61
2	C	401	GRA	C2-C3-C4	-4.77	104.42	112.36
2	B	401	GRA	C2-C3-C4	-4.72	104.50	112.36
2	D	401	GRA	C6-C5-N2	4.46	121.79	112.42
2	B	401	GRA	O4-C7-C8	-4.42	118.77	123.99
2	A	401	GRA	C2-N1-C1	4.36	130.37	122.59
2	A	401	GRA	O4-C7-S1	3.91	127.69	122.61
2	C	401	GRA	C6-S1-C7	3.67	113.28	101.87
2	C	401	GRA	C15-C12-C13	3.65	114.19	108.23
2	B	401	GRA	C3-C2-N1	3.65	119.26	111.90
2	D	401	GRA	C8-C7-S1	3.63	117.68	113.46
2	A	401	GRA	C5-N2-C4	3.56	129.44	122.84
2	A	401	GRA	C9-C8-C7	3.31	119.67	112.33
2	C	401	GRA	O3-C4-C3	-3.26	116.05	122.02
2	C	401	GRA	C5A-C6A-N6A	3.08	125.03	120.35
2	B	401	GRA	O3-C4-C3	-3.04	116.46	122.02
2	B	401	GRA	C6-C5-N2	2.80	118.30	112.42
2	B	401	GRA	C3-C4-N2	2.56	120.73	116.42
2	B	401	GRA	P2A-O3A-P1A	2.50	141.39	132.83
2	A	401	GRA	C5A-C6A-N6A	2.42	124.03	120.35
2	B	401	GRA	O4-C7-S1	2.36	125.68	122.61
2	B	401	GRA	C5A-C6A-N6A	2.35	123.93	120.35
2	B	401	GRA	O5-C11-C10	-2.35	115.52	123.08
2	D	401	GRA	P2A-O3A-P1A	2.35	140.89	132.83
2	D	401	GRA	O4-C7-S1	2.32	125.63	122.61
2	D	401	GRA	C16-C12-C15	-2.23	104.62	109.17
2	C	401	GRA	C16-C12-C14	2.17	112.59	108.82
2	C	401	GRA	C3X-C2X-C1X	2.15	104.64	99.89
2	A	401	GRA	C15-C12-C14	2.07	112.41	108.82
2	B	401	GRA	C10-C9-C8	2.02	116.47	112.19
2	B	401	GRA	O6-C11-C10	2.01	120.50	114.03
2	A	401	GRA	C10-C9-C8	2.01	116.45	112.19

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GRA	C5X-O5X-P1A-O3A
2	A	401	GRA	C13-O6A-P2A-O3A
2	A	401	GRA	C13-O6A-P2A-O4A
2	A	401	GRA	C16-C12-C13-O6A
2	A	401	GRA	C14-C12-C13-O6A
2	A	401	GRA	C13-C12-C14-O1
2	A	401	GRA	C13-C12-C14-C1
2	A	401	GRA	C15-C12-C14-O1
2	A	401	GRA	C15-C12-C14-C1
2	A	401	GRA	C16-C12-C14-O1
2	A	401	GRA	C16-C12-C14-C1
2	A	401	GRA	N1-C1-C14-O1
2	A	401	GRA	N1-C2-C3-C4
2	A	401	GRA	O4-C7-S1-C6
2	A	401	GRA	C8-C7-S1-C6
2	A	401	GRA	C7-C8-C9-C10
2	B	401	GRA	C3X-O3X-P3X-O8A
2	B	401	GRA	C3X-C4X-C5X-O5X
2	B	401	GRA	C5X-O5X-P1A-O1A
2	B	401	GRA	C5X-O5X-P1A-O2A
2	B	401	GRA	C13-O6A-P2A-O3A
2	B	401	GRA	C13-O6A-P2A-O4A
2	B	401	GRA	C13-O6A-P2A-O5A
2	B	401	GRA	O4-C7-S1-C6
2	B	401	GRA	C8-C7-S1-C6
2	C	401	GRA	C3X-C4X-C5X-O5X
2	C	401	GRA	O4X-C4X-C5X-O5X
2	C	401	GRA	C5X-O5X-P1A-O1A
2	C	401	GRA	C5X-O5X-P1A-O2A
2	C	401	GRA	C13-O6A-P2A-O3A
2	C	401	GRA	C13-O6A-P2A-O4A
2	C	401	GRA	C13-O6A-P2A-O5A
2	C	401	GRA	C14-C12-C13-O6A
2	C	401	GRA	C13-C12-C14-C1
2	C	401	GRA	C15-C12-C14-C1
2	C	401	GRA	C14-C1-N1-C2
2	C	401	GRA	C5-C6-S1-C7
2	C	401	GRA	O4-C7-S1-C6
2	C	401	GRA	C8-C7-S1-C6
2	D	401	GRA	C5X-O5X-P1A-O3A

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Mol	Chain	Res	Type	Atoms
2	D	401	GRA	C13-O6A-P2A-O4A
2	D	401	GRA	C13-O6A-P2A-O5A
2	D	401	GRA	C12-C13-O6A-P2A
2	D	401	GRA	C16-C12-C13-O6A
2	D	401	GRA	C14-C12-C13-O6A
2	D	401	GRA	O2-C1-C14-O1
2	D	401	GRA	C14-C1-N1-C2
2	D	401	GRA	C6-C5-N2-C4
2	D	401	GRA	O4-C7-S1-C6
2	D	401	GRA	C8-C7-S1-C6
2	C	401	GRA	O2-C1-N1-C2
2	D	401	GRA	O2-C1-N1-C2
2	B	401	GRA	O4X-C4X-C5X-O5X
2	D	401	GRA	C4X-C3X-O3X-P3X
2	D	401	GRA	C3X-C4X-C5X-O5X
2	D	401	GRA	O4X-C4X-C5X-O5X
2	A	401	GRA	C15-C12-C13-O6A
2	D	401	GRA	C15-C12-C13-O6A
2	A	401	GRA	C11-C10-C9-C8
2	C	401	GRA	N1-C2-C3-C4
2	C	401	GRA	C11-C10-C9-C8
2	A	401	GRA	O2-C1-C14-O1
2	C	401	GRA	O2-C1-C14-O1
2	B	401	GRA	C15-C12-C13-O6A
2	C	401	GRA	C4X-C5X-O5X-P1A
2	C	401	GRA	P1A-O3A-P2A-O6A
2	D	401	GRA	P2A-O3A-P1A-O5X
2	D	401	GRA	P1A-O3A-P2A-O6A
2	B	401	GRA	C7-C8-C9-C10
2	C	401	GRA	N1-C1-C14-O1
2	B	401	GRA	C5X-O5X-P1A-O3A
2	A	401	GRA	C5X-O5X-P1A-O2A
2	A	401	GRA	C13-O6A-P2A-O5A
2	D	401	GRA	C5X-O5X-P1A-O2A
2	A	401	GRA	C4X-C5X-O5X-P1A
2	B	401	GRA	C16-C12-C13-O6A
2	C	401	GRA	C16-C12-C13-O6A
2	B	401	GRA	N1-C2-C3-C4
2	A	401	GRA	O4X-C4X-C5X-O5X
2	C	401	GRA	C4X-C3X-O3X-P3X
2	C	401	GRA	C15-C12-C13-O6A
2	B	401	GRA	C4X-C5X-O5X-P1A

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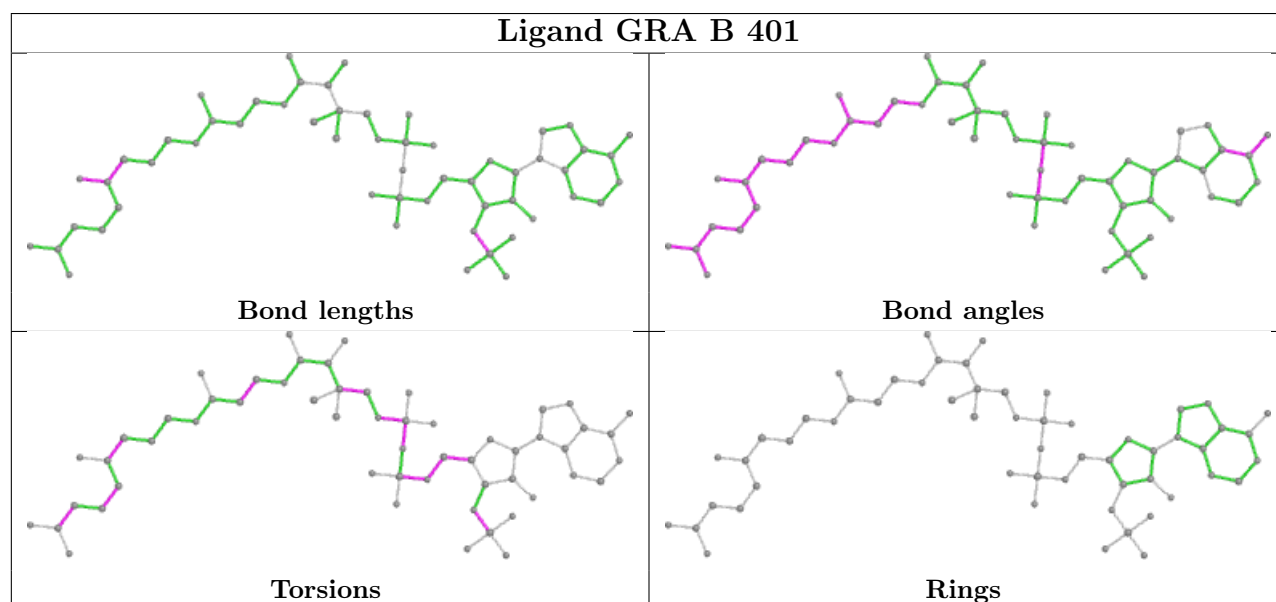
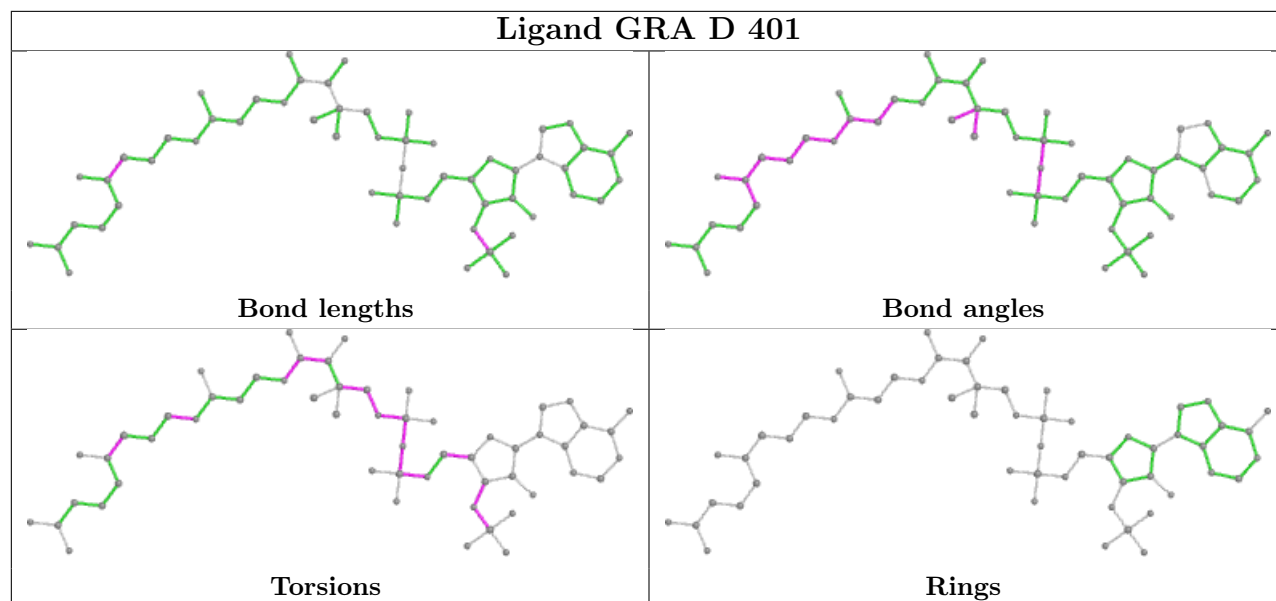
Mol	Chain	Res	Type	Atoms
2	B	401	GRA	C9-C10-C11-O6
2	B	401	GRA	C9-C10-C11-O5
2	C	401	GRA	C3X-O3X-P3X-O8A
2	D	401	GRA	C3X-O3X-P3X-O8A
2	C	401	GRA	C16-C12-C14-C1
2	C	401	GRA	C3X-O3X-P3X-O9A
2	C	401	GRA	C5X-O5X-P1A-O3A
2	D	401	GRA	C3X-O3X-P3X-O9A
2	D	401	GRA	C3X-O3X-P3X-O7A
2	D	401	GRA	C13-O6A-P2A-O3A
2	B	401	GRA	P1A-O3A-P2A-O4A
2	C	401	GRA	P1A-O3A-P2A-O5A
2	C	401	GRA	C12-C13-O6A-P2A
2	C	401	GRA	C9-C10-C11-O6
2	C	401	GRA	C9-C10-C11-O5

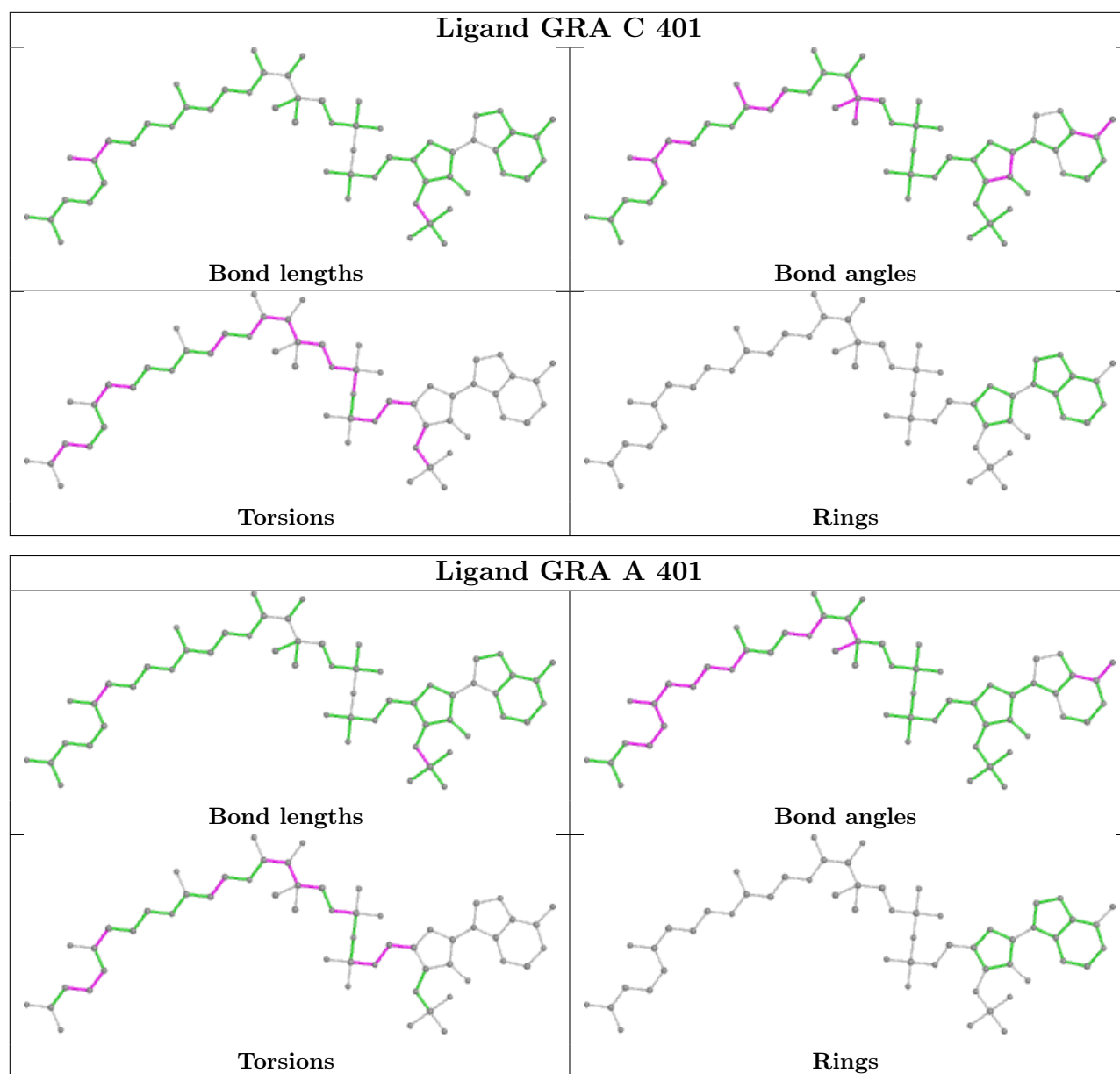
There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	GRA	4	0
2	B	401	GRA	4	0
2	C	401	GRA	3	0
2	A	401	GRA	6	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	326/327 (99%)	0.13	6 (1%) 67 64	20, 42, 71, 87	0
1	B	327/327 (100%)	0.11	9 (2%) 55 51	18, 41, 71, 84	0
1	C	327/327 (100%)	-0.04	9 (2%) 55 51	18, 36, 66, 88	0
1	D	327/327 (100%)	0.98	34 (10%) 13 12	29, 67, 100, 118	0
All	All	1307/1308 (99%)	0.29	58 (4%) 39 36	18, 46, 87, 118	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	PHE	4.3
1	A	209	ILE	3.4
1	D	283	PHE	3.3
1	A	210	ALA	3.2
1	C	210	ALA	3.2
1	D	159	PHE	3.2
1	C	209	ILE	3.2
1	D	41	GLY	3.1
1	D	303	PRO	2.9
1	D	73	ALA	2.9
1	A	38	ARG	2.8
1	D	43	ARG	2.8
1	D	297	ILE	2.8
1	A	3	THR	2.7
1	B	207	GLY	2.7
1	D	160	ALA	2.6
1	D	249	ILE	2.6
1	C	207	GLY	2.6
1	D	282	SER	2.6
1	C	34	GLY	2.6
1	D	204	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	260	ARG	2.6
1	C	38	ARG	2.6
1	D	269	LEU	2.5
1	D	207	GLY	2.5
1	D	17	ALA	2.4
1	D	48	ALA	2.4
1	A	206	ALA	2.4
1	D	25	ILE	2.4
1	D	252	PHE	2.4
1	C	208	MET	2.4
1	C	2	GLN	2.4
1	B	265	VAL	2.3
1	B	206	ALA	2.3
1	D	224	PHE	2.3
1	A	100	ARG	2.3
1	D	247	ALA	2.3
1	B	221	ARG	2.3
1	D	328	VAL	2.3
1	C	221	ARG	2.2
1	D	47	TRP	2.2
1	D	209	ILE	2.2
1	D	29	LEU	2.2
1	B	273	ARG	2.2
1	B	204	PHE	2.2
1	D	205	SER	2.2
1	D	274	GLU	2.2
1	D	270	GLY	2.1
1	B	39	ARG	2.1
1	B	246	ALA	2.1
1	B	240	HIS	2.1
1	D	23	ALA	2.1
1	D	284	GLY	2.1
1	D	300	ALA	2.1
1	D	306	GLY	2.1
1	D	11	PHE	2.0
1	D	2	GLN	2.0
1	D	61	ALA	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](#)

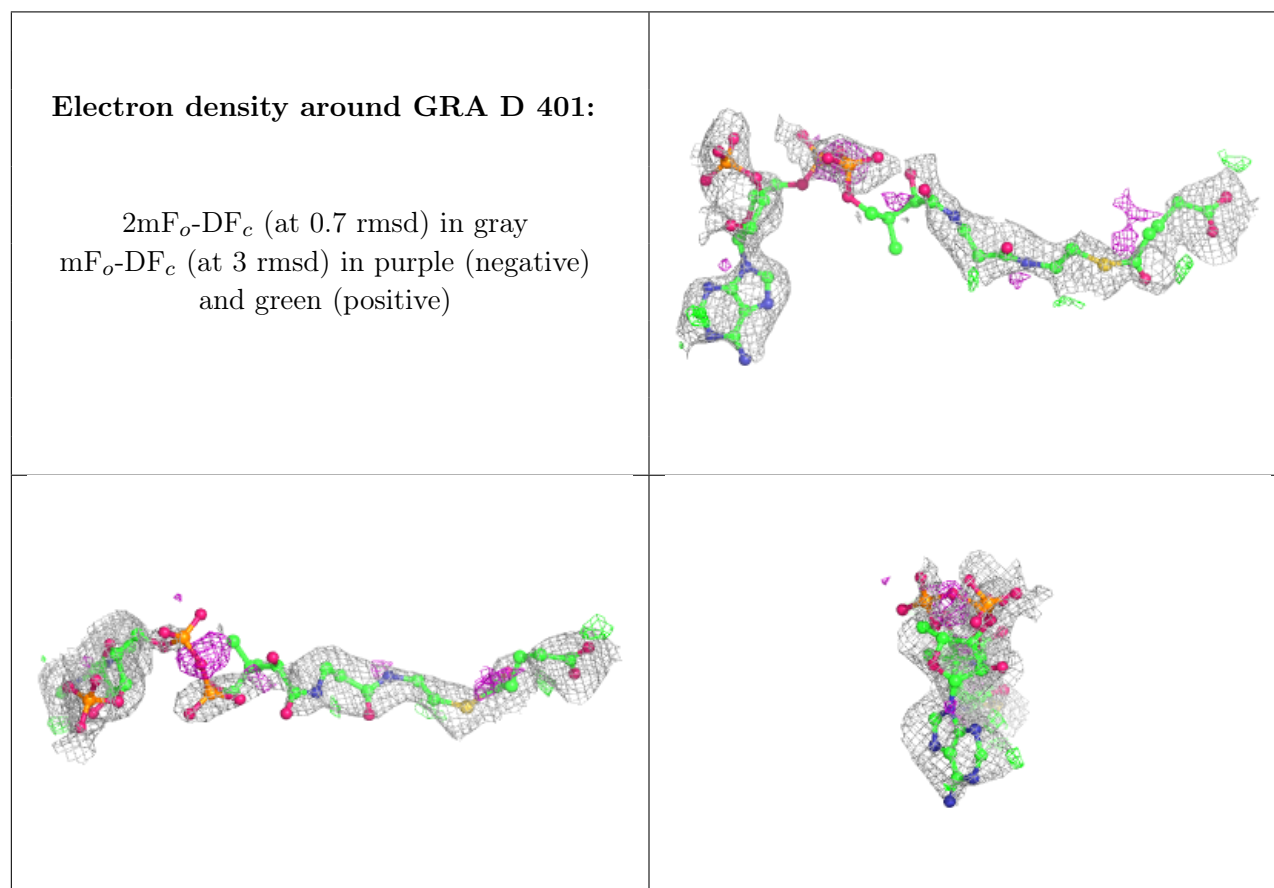
There are no oligosaccharides in this entry.

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.

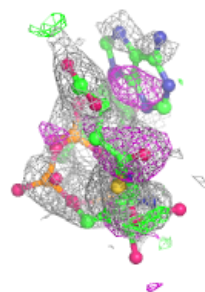
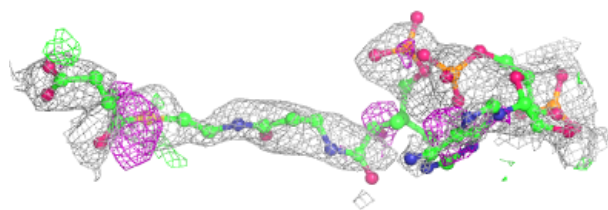
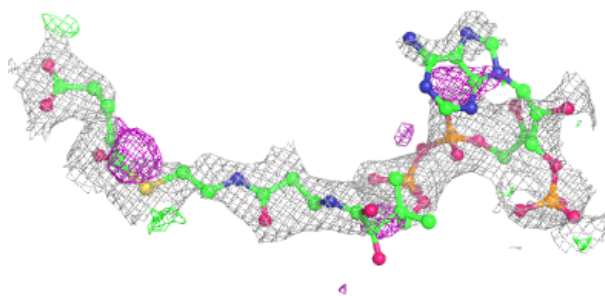
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GRA	D	401	56/56	0.64	0.19	37,98,141,149	0
2	GRA	C	401	56/56	0.72	0.21	26,105,140,141	0
2	GRA	B	401	56/56	0.75	0.20	24,108,152,154	0
2	GRA	A	401	56/56	0.77	0.18	22,93,151,153	0

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.

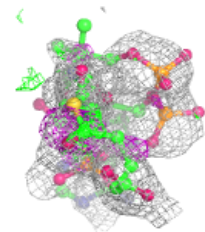
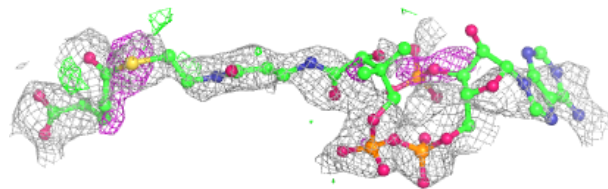
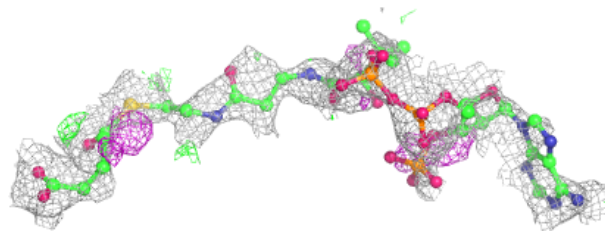


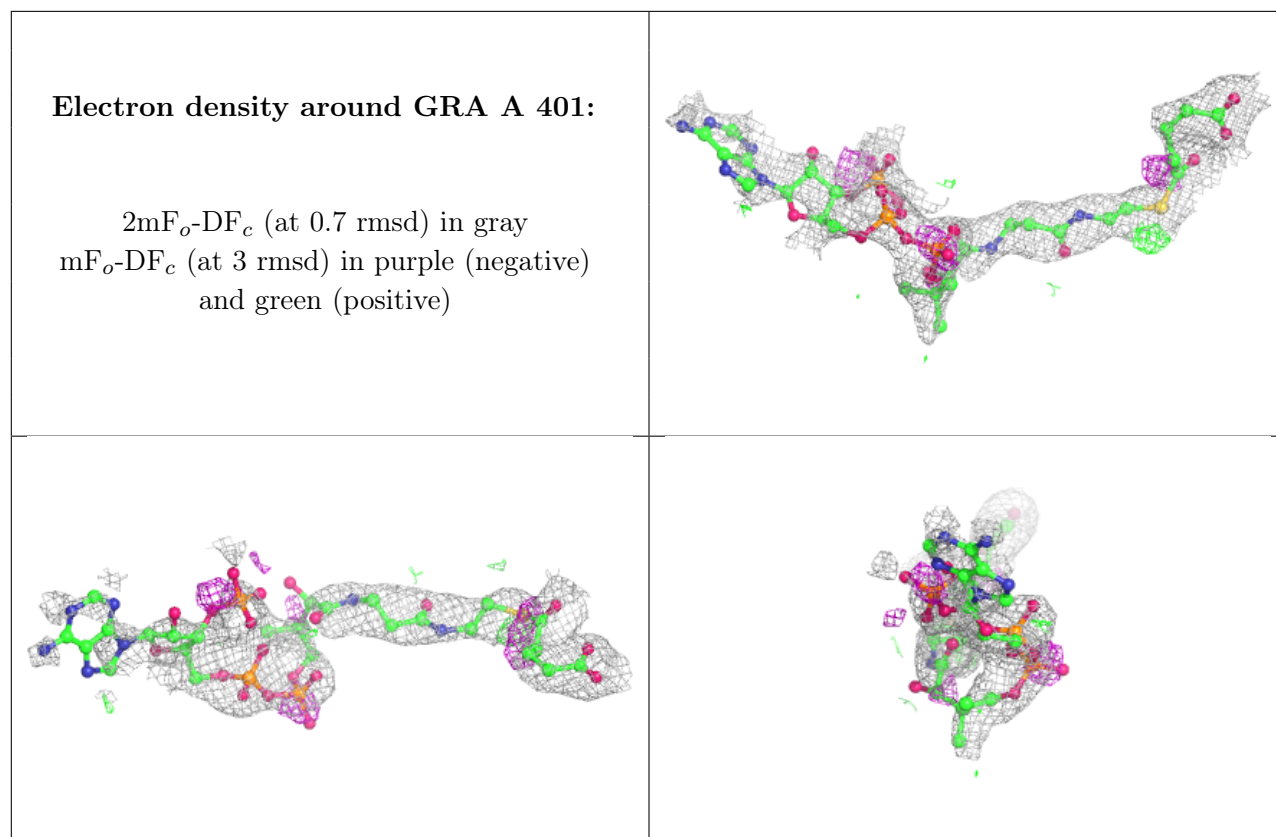
Electron density around GRA C 401:

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

**Electron density around GRA B 401:**

$2mF_o-DF_c$ (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.