



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:58 pm BST

PDB ID : 3CC9
Title : Crystal structure of Plasmodium vivax putative polyprenyl pyrophosphate synthase in complex with geranylgeranyl diphosphate
Authors : Wernimont, A.K.; Dunford, J.; Lew, J.; Zhao, Y.; Koziaradzki, I.; Cossar, D.; Schapira, M.; Bochkarev, A.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Hui, R.; Artz, J.D.; Structural Genomics Consortium (SGC)
Deposited on : 2008-02-25
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

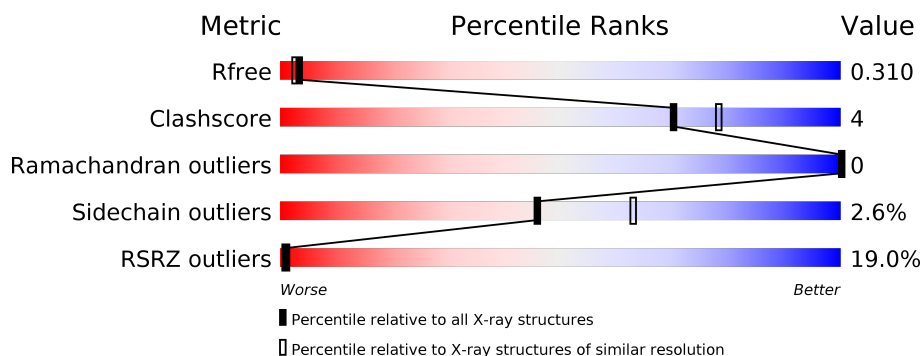
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	396	<div> <div>13%</div> <div>74%</div> <div>11%</div> <div>•</div> <div>13%</div> </div>
1	B	396	<div> <div>13%</div> <div>84%</div> <div>7%</div> <div>10%</div> </div>
1	C	396	<div> <div>25%</div> <div>76%</div> <div>8%</div> <div>16%</div> </div>
1	D	396	<div> <div>15%</div> <div>79%</div> <div>6%</div> <div>•</div> <div>15%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11221 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 Putative farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	1	0
			2764	1793	439	517	15			
1	B	358	Total	C	N	O	S	0	2	0
			2885	1873	462	535	15			
1	C	332	Total	C	N	O	S	0	0	0
			2578	1663	420	481	14			
1	D	337	Total	C	N	O	S	0	0	0
			2639	1702	423	499	15			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP A5K4U6
A	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	3	SER	-	EXPRESSION TAG	UNP A5K4U6
A	4	SER	-	EXPRESSION TAG	UNP A5K4U6
A	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	11	SER	-	EXPRESSION TAG	UNP A5K4U6
A	12	SER	-	EXPRESSION TAG	UNP A5K4U6
A	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
A	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
A	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
A	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
A	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
A	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
A	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
A	21	GLY	-	EXPRESSION TAG	UNP A5K4U6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	134	MET	THR	SEE REMARK 999	UNP A5K4U6
A	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
B	1	MET	-	EXPRESSION TAG	UNP A5K4U6
B	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	3	SER	-	EXPRESSION TAG	UNP A5K4U6
B	4	SER	-	EXPRESSION TAG	UNP A5K4U6
B	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	11	SER	-	EXPRESSION TAG	UNP A5K4U6
B	12	SER	-	EXPRESSION TAG	UNP A5K4U6
B	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
B	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
B	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
B	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
B	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
B	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
B	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
B	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	134	MET	THR	SEE REMARK 999	UNP A5K4U6
B	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
C	1	MET	-	EXPRESSION TAG	UNP A5K4U6
C	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	3	SER	-	EXPRESSION TAG	UNP A5K4U6
C	4	SER	-	EXPRESSION TAG	UNP A5K4U6
C	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	11	SER	-	EXPRESSION TAG	UNP A5K4U6
C	12	SER	-	EXPRESSION TAG	UNP A5K4U6
C	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
C	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
C	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
C	17	LEU	-	EXPRESSION TAG	UNP A5K4U6

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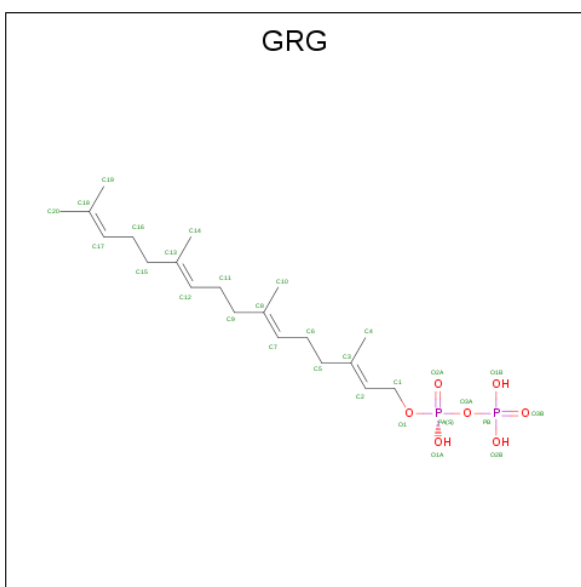
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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
C	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
C	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
C	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	134	MET	THR	SEE REMARK 999	UNP A5K4U6
C	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
D	1	MET	-	EXPRESSION TAG	UNP A5K4U6
D	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	3	SER	-	EXPRESSION TAG	UNP A5K4U6
D	4	SER	-	EXPRESSION TAG	UNP A5K4U6
D	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	11	SER	-	EXPRESSION TAG	UNP A5K4U6
D	12	SER	-	EXPRESSION TAG	UNP A5K4U6
D	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
D	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
D	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
D	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
D	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
D	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
D	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
D	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	134	MET	THR	SEE REMARK 999	UNP A5K4U6
D	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is GERANYLGERANYL DIPHOSPHATE (three-letter code: GRG) (formula: C₂₀H₃₆O₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 29	C 20	O 7	P 2	0	0
3	B	1	Total 29	C 20	O 7	P 2	0	0
3	C	1	Total 27	C 18	O 7	P 2	0	0
3	D	1	Total 29	C 20	O 7	P 2	0	0

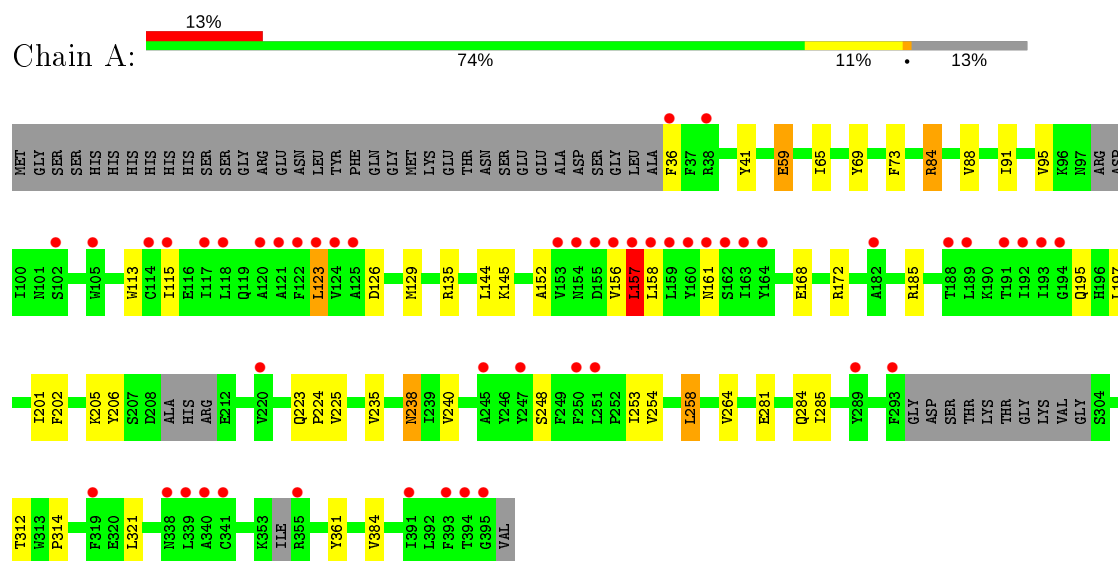
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	75	Total O 75 75	0	0
4	B	83	Total O 83 83	0	0
4	C	47	Total O 47 47	0	0
4	D	35	Total O 35 35	0	0

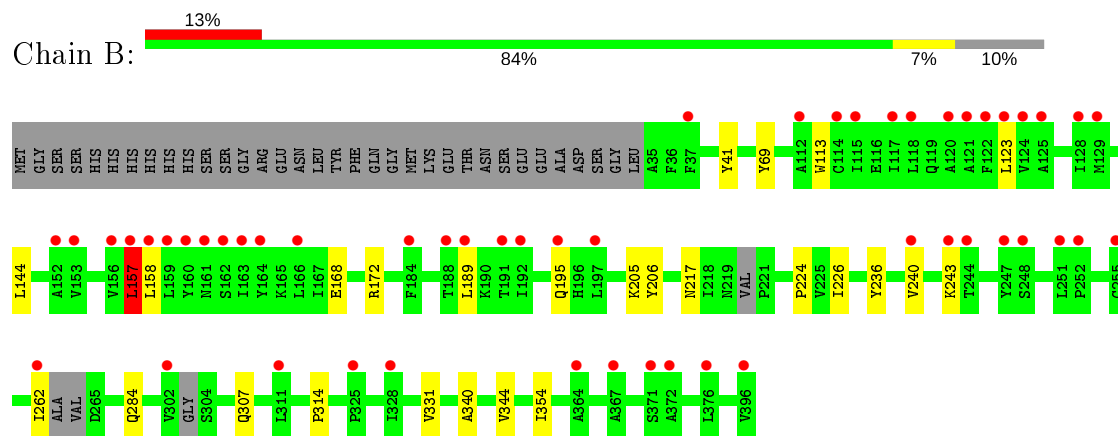
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

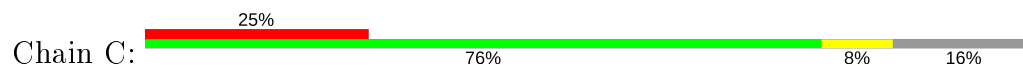
- Molecule 1: Putative farnesyl pyrophosphate synthase

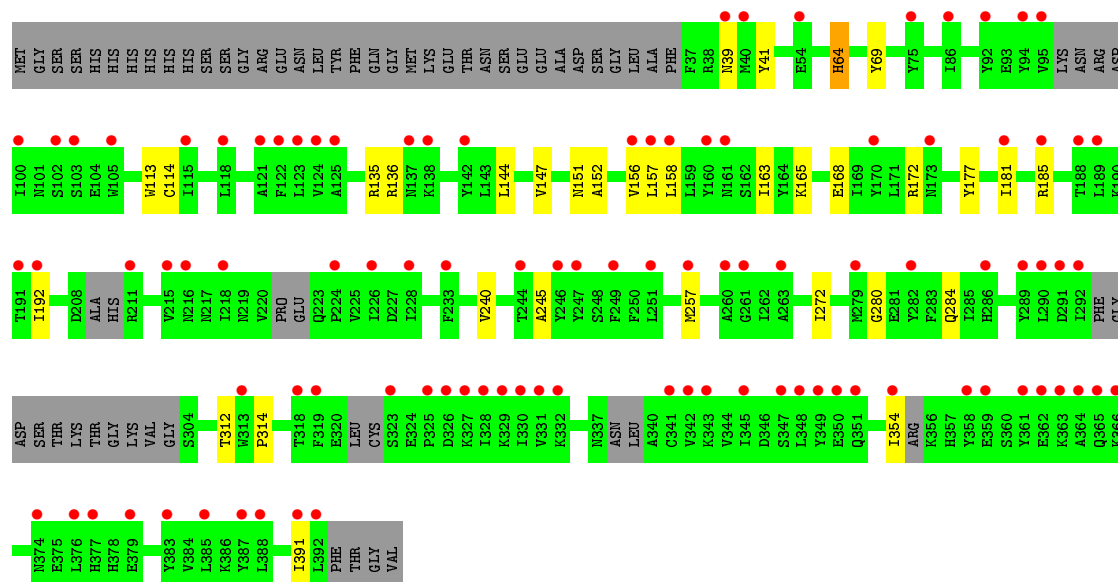


- Molecule 1: Putative farnesyl pyrophosphate synthase

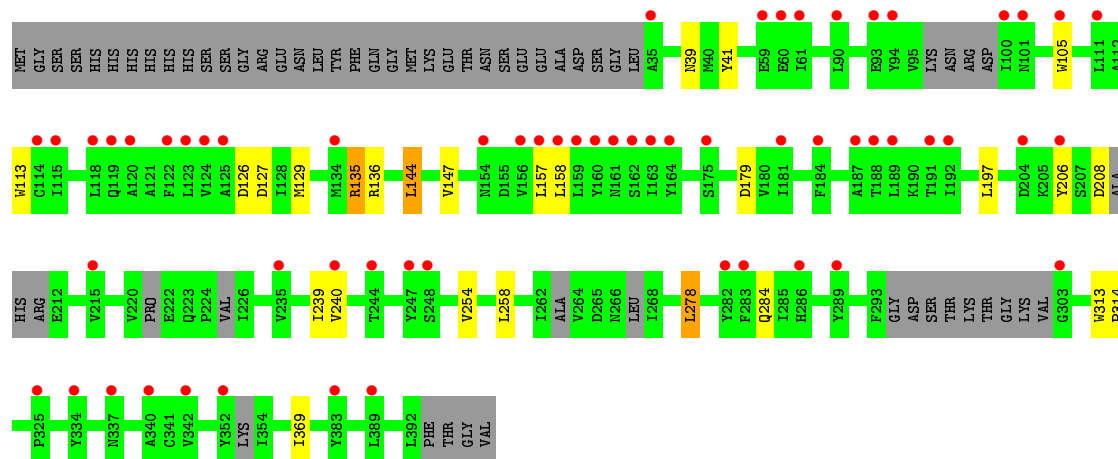
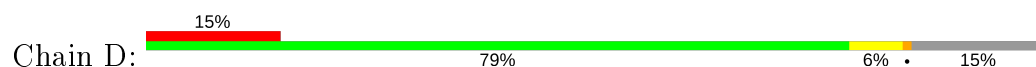


- Molecule 1: Putative farnesyl pyrophosphate synthase





• Molecule 1: Putative farnesyl pyrophosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.09Å 108.98Å 141.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.61 – 2.30 34.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.61-2.30) 99.7 (34.40-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.296 0.275 , 0.310	Depositor DCC
R_{free} test set	3720 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11221	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: GRG, NA

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	0.36	0/2821	0.54	3/3829 (0.1%)
1	B	0.38	0/2952	0.53	2/3999 (0.1%)
1	C	0.33	0/2626	0.46	0/3569
1	D	0.34	0/2687	0.49	0/3644
All	All	0.36	0/11086	0.51	5/15041 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	LEU	CA-CB-CG	-5.83	101.88	115.30
1	A	84	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	123	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	157	LEU	CA-CB-CG	-5.41	102.85	115.30
1	B	123	LEU	CA-CB-CG	5.29	127.46	115.30

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	2764	0	2595	31	0
1	B	2885	0	2749	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2578	0	2319	17	0
1	D	2639	0	2417	14	0
2	A	1	0	0	0	0
3	A	29	0	21	2	0
3	B	29	0	21	2	0
3	C	27	0	15	0	0
3	D	29	0	23	1	0
4	A	75	0	0	0	0
4	B	83	0	0	1	0
4	C	47	0	0	1	0
4	D	35	0	0	0	0
All	All	11221	0	10160	75	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 4.

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASN:HB3	1:B:189:LEU:HD11	1.71	0.73
1:A:161:ASN:HB3	1:B:189:LEU:CD1	2.19	0.72
1:A:157:LEU:HD22	3:B:501:GRG:H203	1.73	0.71
1:D:127:ASP:OD2	1:D:135:ARG:HG3	1.92	0.69
1:A:84:ARG:NH1	3:A:501:GRG:O2A	2.25	0.68
1:A:168:GLU:O	1:A:172:ARG:HB2	1.95	0.67
1:A:59[A]:GLU:H	1:A:59[A]:GLU:CD	1.98	0.67
1:A:129:MET:CE	1:A:195:GLN:HE21	2.09	0.64
1:D:240:VAL:HG22	1:D:284:GLN:HG2	1.77	0.64
1:B:205:LYS:HG3	1:B:206:TYR:HD2	1.63	0.62
1:B:168:GLU:O	1:B:172:ARG:HB2	1.99	0.62
1:A:240:VAL:HG22	1:A:284:GLN:HG2	1.84	0.60
1:B:240:VAL:HG22	1:B:284:GLN:HG2	1.84	0.58
1:A:91:ILE:O	1:A:95:VAL:HG22	2.05	0.56
1:A:91:ILE:HD13	1:A:253:ILE:HA	1.87	0.56
1:A:240:VAL:HG11	1:A:281:GLU:HA	1.88	0.56
1:C:257:MET:SD	1:C:272:ILE:HD13	2.46	0.55
1:A:145:LYS:HD2	1:B:217:ASN:ND2	2.21	0.54
1:C:41:TYR:HB2	1:C:113:TRP:CZ2	2.43	0.54
1:D:41:TYR:HB2	1:D:113:TRP:CZ2	2.43	0.54
1:C:192:ILE:HG21	1:D:158:LEU:HB2	1.90	0.53
1:B:205:LYS:HG3	1:B:206:TYR:CD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:GLN:HE21	1:B:243:LYS:HD2	1.75	0.51
1:B:41:TYR:HB2	1:B:113:TRP:CZ2	2.46	0.51
1:C:168:GLU:O	1:C:172:ARG:HB3	2.10	0.51
1:C:312:THR:HB	1:C:314:PRO:HD2	1.92	0.51
1:C:136:ARG:HD2	4:C:528:HOH:O	2.11	0.50
1:A:91:ILE:HG13	1:A:384:VAL:HG11	1.92	0.50
1:A:129:MET:HE1	1:A:195:GLN:HE21	1.77	0.49
1:A:84:ARG:HD3	1:A:248:SER:HA	1.94	0.49
1:A:254:VAL:O	1:A:258:LEU:HB2	2.12	0.49
1:C:240:VAL:HG22	1:C:284:GLN:HG2	1.95	0.49
1:D:136:ARG:HD2	3:D:501:GRG:O2B	2.13	0.49
1:B:226:ILE:HD11	1:B:331:VAL:HG22	1.95	0.49
1:D:278:LEU:HB3	1:D:369:ILE:HG12	1.94	0.48
3:A:501:GRG:H203	1:B:157:LEU:HD22	1.95	0.48
1:C:245:ALA:HB2	1:C:280:GLY:HA3	1.96	0.48
1:A:205:LYS:HG3	1:A:206:TYR:HD2	1.79	0.48
1:C:64:HIS:CD2	1:D:206:TYR:HA	2.48	0.47
1:D:254:VAL:O	1:D:258:LEU:HB2	2.13	0.47
1:A:41:TYR:HB2	1:A:113:TRP:CZ2	2.50	0.47
1:D:144:LEU:HB2	1:D:147:VAL:HG12	1.97	0.47
1:A:202:PHE:HB3	1:A:225:VAL:O	2.15	0.46
1:A:312:THR:HB	1:A:314:PRO:HD2	1.98	0.46
1:C:69:TYR:CE1	1:C:158:LEU:HD22	2.49	0.46
1:C:69:TYR:CD1	1:C:158:LEU:HD22	2.51	0.46
1:B:340:ALA:O	1:B:344:VAL:HG23	2.16	0.46
1:D:126:ASP:HA	1:D:129:MET:HE3	1.98	0.45
1:B:69:TYR:CE1	1:B:158:LEU:HD22	2.52	0.44
1:C:314:PRO:HB3	1:C:354:ILE:HG21	1.99	0.44
1:B:314:PRO:HB3	1:B:354:ILE:HG21	2.00	0.44
1:C:152:ALA:O	1:C:156:VAL:HG23	2.17	0.44
1:D:144:LEU:HB2	1:D:147:VAL:CG1	2.47	0.44
1:B:69:TYR:CD1	1:B:158:LEU:HD22	2.53	0.44
1:C:177:TYR:CZ	1:C:181:ILE:HD11	2.53	0.44
1:A:152:ALA:O	1:A:156:VAL:HG23	2.18	0.43
1:B:195:GLN:CG	3:B:501:GRG:HC91	2.49	0.43
1:C:114:CYS:HB3	1:C:163:ILE:HG23	2.00	0.43
1:A:88:VAL:HG21	1:A:115:ILE:HD12	2.01	0.43
1:A:69:TYR:CD1	1:A:158:LEU:HD22	2.54	0.43
1:A:91:ILE:CD1	1:A:253:ILE:HG12	2.49	0.42
1:B:236:TYR:CZ	1:B:240:VAL:HG21	2.54	0.42
1:A:223:GLN:HA	1:A:224:PRO:HD3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:VAL:O	1:C:151:ASN:HB2	2.19	0.42
1:A:197:LEU:O	1:A:201:ILE:HB	2.19	0.42
1:D:313:TRP:HB3	1:D:314:PRO:HD3	2.01	0.42
1:A:285:ILE:HD12	1:A:361:TYR:CZ	2.55	0.41
1:A:126:ASP:HA	1:A:129:MET:HE3	2.03	0.41
1:A:69:TYR:O	1:A:73:PHE:HD2	2.03	0.41
1:C:391:ILE:O	1:C:391:ILE:HG22	2.21	0.41
1:A:123:LEU:HG	1:A:135:ARG:HG2	2.03	0.40
1:D:179:ASP:HB3	1:D:258:LEU:HD21	2.02	0.40
1:D:197:LEU:HB3	1:D:239:ILE:HG12	2.03	0.40
1:B:224:PRO:HA	4:B:581:HOH:O	2.21	0.40
1:A:235:VAL:O	1:A:238:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/396 (85%)	329 (98%)	6 (2%)	0	100	100
1	B	352/396 (89%)	341 (97%)	11 (3%)	0	100	100
1	C	316/396 (80%)	308 (98%)	8 (2%)	0	100	100
1	D	319/396 (81%)	308 (97%)	11 (3%)	0	100	100
All	All	1322/1584 (84%)	1286 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	277/357 (78%)	266 (96%)	11 (4%)	31	44
1	B	294/357 (82%)	290 (99%)	4 (1%)	67	81
1	C	235/357 (66%)	228 (97%)	7 (3%)	41	57
1	D	255/357 (71%)	248 (97%)	7 (3%)	44	61
All	All	1061/1428 (74%)	1032 (97%)	29 (3%)	46	61

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	PHE
1	A	59[A]	GLU
1	A	59[B]	GLU
1	A	65	ILE
1	A	144	LEU
1	A	157	LEU
1	A	185	ARG
1	A	238	ASN
1	A	258	LEU
1	A	264	VAL
1	A	321	LEU
1	B	144	LEU
1	B	157	LEU
1	B	262	ILE
1	B	307	GLN
1	C	39	ASN
1	C	64	HIS
1	C	135	ARG
1	C	144	LEU
1	C	157	LEU
1	C	165	LYS
1	C	185	ARG
1	D	39	ASN
1	D	105	TRP
1	D	135	ARG
1	D	144	LEU
1	D	157	LEU
1	D	208	ASP

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Mol	Chain	Res	Type
1	D	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	ASN
1	C	64	HIS
1	C	82	ASN
1	C	173	ASN
1	D	195	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is 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
3	GRG	D	501	-	26,28,28	2.96	7 (26%)	33,37,37	6.54	10 (30%)
3	GRG	A	501	-	26,28,28	3.02	7 (26%)	33,37,37	7.36	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GRG	C	501	-	24,26,28	3.12	7 (29%)	30,34,37	7.97	11 (36%)
3	GRG	B	501	-	26,28,28	2.99	7 (26%)	33,37,37	6.90	12 (36%)

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	GRG	D	501	-	-	10/31/31/31	-
3	GRG	A	501	-	-	11/31/31/31	-
3	GRG	C	501	-	-	14/29/29/31	-
3	GRG	B	501	-	-	13/31/31/31	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	GRG	C1-C2	-7.82	1.25	1.49
3	A	501	GRG	C1-C2	-7.69	1.26	1.49
3	C	501	GRG	C11-C12	-7.50	1.26	1.50
3	C	501	GRG	C6-C7	-7.46	1.26	1.50
3	D	501	GRG	C11-C12	-7.44	1.26	1.50
3	A	501	GRG	C11-C12	-7.41	1.26	1.50
3	B	501	GRG	C6-C7	-7.35	1.26	1.50
3	D	501	GRG	C1-C2	-7.28	1.27	1.49
3	B	501	GRG	C1-C2	-7.20	1.27	1.49
3	A	501	GRG	C6-C7	-7.18	1.27	1.50
3	B	501	GRG	C11-C12	-6.99	1.27	1.50
3	D	501	GRG	C6-C7	-6.82	1.28	1.50
3	B	501	GRG	C16-C17	-6.79	1.28	1.50
3	D	501	GRG	C16-C17	-6.33	1.29	1.50
3	A	501	GRG	C16-C17	-6.29	1.29	1.50
3	C	501	GRG	C16-C17	-5.34	1.26	1.49
3	C	501	GRG	C2-C3	-2.96	1.25	1.33
3	C	501	GRG	C7-C8	-2.94	1.26	1.33
3	D	501	GRG	C12-C13	-2.93	1.26	1.33
3	C	501	GRG	C12-C13	-2.90	1.26	1.33
3	D	501	GRG	C2-C3	-2.88	1.26	1.33
3	A	501	GRG	C7-C8	-2.85	1.26	1.33
3	A	501	GRG	C12-C13	-2.85	1.26	1.33
3	D	501	GRG	C7-C8	-2.78	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GRG	C2-C3	-2.78	1.26	1.33
3	B	501	GRG	C7-C8	-2.73	1.26	1.33
3	B	501	GRG	C2-C3	-2.70	1.26	1.33
3	B	501	GRG	C12-C13	-2.53	1.26	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GRG	C1-C2-C3	30.63	179.02	126.04
3	C	501	GRG	C1-C2-C3	30.32	178.49	126.04
3	B	501	GRG	C1-C2-C3	25.27	169.74	126.04
3	D	501	GRG	C1-C2-C3	24.21	167.91	126.04
3	C	501	GRG	C6-C7-C8	21.41	179.21	127.66
3	C	501	GRG	C11-C12-C13	19.88	175.53	127.66
3	D	501	GRG	C11-C12-C13	19.83	175.41	127.66
3	B	501	GRG	C11-C12-C13	19.12	173.70	127.66
3	A	501	GRG	C11-C12-C13	18.82	172.97	127.66
3	B	501	GRG	C6-C7-C8	18.47	172.14	127.66
3	A	501	GRG	C6-C7-C8	17.44	169.65	127.66
3	D	501	GRG	C6-C7-C8	15.73	165.54	127.66
3	B	501	GRG	C16-C17-C18	11.48	166.98	127.75
3	D	501	GRG	C16-C17-C18	9.96	161.79	127.75
3	A	501	GRG	C16-C17-C18	9.91	161.60	127.75
3	C	501	GRG	C16-C17-C18	6.65	172.04	126.84
3	C	501	GRG	C4-C3-C5	4.21	122.36	115.27
3	B	501	GRG	C4-C3-C5	4.02	122.03	115.27
3	A	501	GRG	C15-C16-C17	3.85	124.54	111.88
3	B	501	GRG	C15-C16-C17	3.68	123.97	111.88
3	D	501	GRG	C4-C3-C5	3.56	121.26	115.27
3	A	501	GRG	C4-C3-C5	3.54	121.23	115.27
3	D	501	GRG	C14-C13-C15	3.54	121.23	115.27
3	C	501	GRG	C14-C13-C15	3.45	121.08	115.27
3	A	501	GRG	C14-C13-C15	3.41	121.01	115.27
3	D	501	GRG	C15-C16-C17	3.32	122.79	111.88
3	C	501	GRG	C15-C16-C17	3.13	120.67	112.63
3	B	501	GRG	C10-C8-C9	3.03	120.36	115.27
3	A	501	GRG	C10-C8-C9	2.95	120.23	115.27
3	B	501	GRG	C9-C11-C12	2.86	121.28	111.88
3	C	501	GRG	C10-C8-C9	2.85	120.06	115.27
3	D	501	GRG	C10-C8-C9	2.83	120.03	115.27
3	C	501	GRG	C5-C6-C7	2.67	120.66	111.88
3	B	501	GRG	C14-C13-C15	2.66	119.75	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	GRG	C9-C11-C12	2.66	120.63	111.88
3	D	501	GRG	C9-C11-C12	2.48	120.03	111.88
3	A	501	GRG	O1-C1-C2	2.39	119.62	109.59
3	B	501	GRG	C4-C3-C2	-2.36	117.61	123.68
3	B	501	GRG	C10-C8-C7	-2.36	117.63	123.68
3	B	501	GRG	PA-O3A-PB	-2.35	124.76	132.83
3	A	501	GRG	C9-C11-C12	2.33	119.55	111.88
3	C	501	GRG	O1-C1-C2	2.21	118.88	109.59
3	D	501	GRG	PA-O3A-PB	-2.16	125.42	132.83
3	A	501	GRG	C10-C8-C7	-2.14	118.19	123.68
3	A	501	GRG	C14-C13-C12	-2.12	118.23	123.68

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	GRG	C11-C12-C13-C14
3	D	501	GRG	C11-C12-C13-C15
3	A	501	GRG	C11-C12-C13-C15
3	A	501	GRG	C4-C3-C5-C6
3	A	501	GRG	C2-C3-C5-C6
3	A	501	GRG	C1-C2-C3-C5
3	A	501	GRG	C1-C2-C3-C4
3	B	501	GRG	C16-C17-C18-C19
3	B	501	GRG	C6-C7-C8-C9
3	B	501	GRG	C6-C7-C8-C10
3	B	501	GRG	C4-C3-C5-C6
3	B	501	GRG	C2-C3-C5-C6
3	B	501	GRG	C1-C2-C3-C5
3	B	501	GRG	C1-C2-C3-C4
3	B	501	GRG	O1-C1-C2-C3
3	C	501	GRG	C11-C12-C13-C14
3	C	501	GRG	C11-C12-C13-C15
3	C	501	GRG	C6-C7-C8-C9
3	C	501	GRG	C6-C7-C8-C10
3	C	501	GRG	C1-C2-C3-C5
3	C	501	GRG	C1-C2-C3-C4
3	C	501	GRG	C1-O1-PA-O2A
3	B	501	GRG	C16-C17-C18-C20
3	D	501	GRG	C6-C7-C8-C10
3	A	501	GRG	C11-C12-C13-C14
3	A	501	GRG	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
3	B	501	GRG	C11-C12-C13-C14
3	D	501	GRG	C6-C7-C8-C9
3	A	501	GRG	C6-C7-C8-C9
3	B	501	GRG	C11-C12-C13-C15
3	C	501	GRG	C4-C3-C5-C6
3	C	501	GRG	C2-C3-C5-C6
3	A	501	GRG	C12-C11-C9-C8
3	A	501	GRG	C3-C5-C6-C7
3	C	501	GRG	C3-C5-C6-C7
3	D	501	GRG	C12-C11-C9-C8
3	B	501	GRG	C12-C11-C9-C8
3	C	501	GRG	C12-C11-C9-C8
3	B	501	GRG	C13-C15-C16-C17
3	D	501	GRG	C4-C3-C5-C6
3	D	501	GRG	C2-C3-C5-C6
3	D	501	GRG	PA-O3A-PB-O2B
3	C	501	GRG	C1-O1-PA-O1A
3	C	501	GRG	C15-C16-C17-C18
3	D	501	GRG	C1-C2-C3-C4
3	C	501	GRG	C1-O1-PA-O3A
3	A	501	GRG	PB-O3A-PA-O1A
3	D	501	GRG	C5-C6-C7-C8

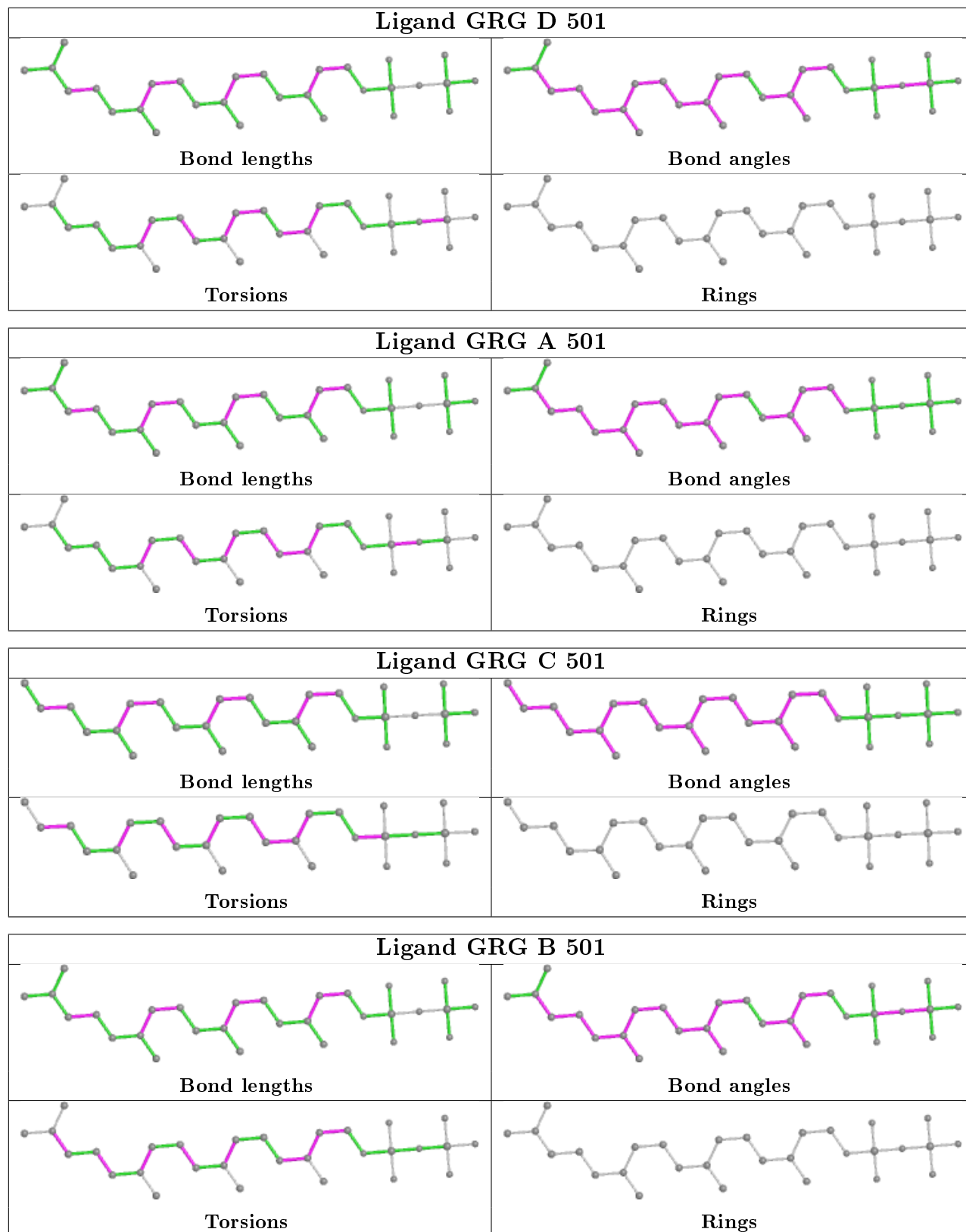
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	GRG	1	0
3	A	501	GRG	2	0
3	B	501	GRG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	344/396 (86%)	0.74	50 (14%) 2 3	45, 57, 70, 76	1 (0%)
1	B	358/396 (90%)	0.75	52 (14%) 2 3	45, 57, 70, 80	0
1	C	332/396 (83%)	1.33	99 (29%) 0 0	49, 65, 77, 91	0
1	D	337/396 (85%)	0.91	60 (17%) 1 1	50, 61, 77, 110	0
All	All	1371/1584 (86%)	0.93	261 (19%) 1 1	45, 59, 75, 110	1 (0%)

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	TYR	7.1
1	D	206	TYR	6.8
1	C	330	ILE	6.2
1	C	354	ILE	5.7
1	C	325	PRO	5.6
1	C	290	LEU	5.4
1	C	342	VAL	5.4
1	A	394	THR	5.1
1	C	94	TYR	5.0
1	A	158	LEU	5.0
1	B	160	TYR	4.9
1	C	383	TYR	4.9
1	A	157	LEU	4.9
1	C	318	THR	4.9
1	C	358	TYR	4.8
1	C	341	CYS	4.8
1	C	102	SER	4.7
1	D	105	TRP	4.6
1	D	191	THR	4.6
1	B	192	ILE	4.6
1	C	192	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	215	VAL	4.5
1	D	192	ILE	4.4
1	C	313	TRP	4.4
1	C	328	ILE	4.3
1	D	157	LEU	4.3
1	C	345	ILE	4.2
1	C	170	TYR	4.1
1	B	191	THR	4.1
1	C	361	TYR	4.1
1	A	395	GLY	4.1
1	D	160	TYR	4.0
1	A	192	ILE	4.0
1	C	347	SER	4.0
1	D	134	MET	3.9
1	C	291	ASP	3.9
1	B	124	VAL	3.9
1	B	158	LEU	3.9
1	C	218	ILE	3.9
1	D	158	LEU	3.9
1	D	101	ASN	3.8
1	C	319	PHE	3.8
1	D	162	SER	3.8
1	B	118	LEU	3.8
1	A	156	VAL	3.8
1	B	120	ALA	3.7
1	C	326	ASP	3.7
1	A	338	ASN	3.6
1	B	157	LEU	3.6
1	C	331	VAL	3.6
1	C	391	ILE	3.6
1	C	157	LEU	3.6
1	C	379	GLU	3.5
1	A	160	TYR	3.5
1	C	188	THR	3.5
1	A	293	PHE	3.5
1	D	159	LEU	3.5
1	C	115	ILE	3.4
1	D	175	SER	3.4
1	C	365	GLN	3.4
1	A	154	ASN	3.4
1	D	115	ILE	3.4
1	C	363	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	247	TYR	3.4
1	A	117	ILE	3.4
1	A	153	VAL	3.3
1	A	159	LEU	3.3
1	B	117	ILE	3.3
1	A	124	VAL	3.3
1	A	355	ARG	3.3
1	C	323	SER	3.3
1	A	121	ALA	3.3
1	A	36	PHE	3.3
1	A	122	PHE	3.3
1	A	319	PHE	3.3
1	C	244	THR	3.3
1	C	121	ALA	3.2
1	A	102	SER	3.2
1	A	105	TRP	3.2
1	B	115	ILE	3.2
1	C	158	LEU	3.2
1	D	122	PHE	3.2
1	D	383	TYR	3.2
1	B	156	VAL	3.2
1	C	376	LEU	3.2
1	D	118	LEU	3.2
1	A	339	LEU	3.2
1	B	122	PHE	3.1
1	A	391	ILE	3.1
1	A	118	LEU	3.1
1	D	244	THR	3.1
1	C	377	HIS	3.1
1	A	393	PHE	3.1
1	C	122	PHE	3.1
1	C	359	GLU	3.0
1	D	352	TYR	3.0
1	B	188	THR	3.0
1	D	342	VAL	3.0
1	A	220	VAL	3.0
1	D	334	TYR	3.0
1	C	92	TYR	3.0
1	A	189	LEU	3.0
1	D	120	ALA	3.0
1	C	161	ASN	2.9
1	B	163	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	105	TRP	2.9
1	C	75	TYR	2.9
1	B	153	VAL	2.9
1	D	163	ILE	2.8
1	D	94	TYR	2.8
1	A	123	LEU	2.8
1	D	184	PHE	2.8
1	C	86	ILE	2.8
1	D	100	ILE	2.8
1	C	279	MET	2.8
1	A	194	GLY	2.8
1	B	248	SER	2.8
1	C	189	LEU	2.8
1	C	350	GLU	2.8
1	A	164	TYR	2.8
1	B	244	THR	2.7
1	A	115	ILE	2.7
1	D	337	ASN	2.7
1	C	351	GLN	2.7
1	D	114	CYS	2.7
1	B	123	LEU	2.7
1	B	252	PRO	2.7
1	B	164	TYR	2.7
1	A	114	CYS	2.7
1	C	233	PHE	2.7
1	D	235	VAL	2.7
1	D	240	VAL	2.7
1	B	189	LEU	2.7
1	D	123	LEU	2.7
1	B	152	ALA	2.6
1	C	124	VAL	2.6
1	D	161	ASN	2.6
1	B	396	VAL	2.6
1	D	164	TYR	2.6
1	D	248	SER	2.6
1	A	125	ALA	2.6
1	C	263	ALA	2.6
1	C	387	TYR	2.6
1	D	156	VAL	2.6
1	B	125	ALA	2.6
1	B	162	SER	2.6
1	D	154	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	260	ALA	2.6
1	D	188	THR	2.6
1	A	341	CYS	2.6
1	C	40	MET	2.6
1	D	124	VAL	2.6
1	C	125	ALA	2.6
1	A	193	ILE	2.6
1	B	37	PHE	2.5
1	C	332	LYS	2.5
1	D	247	TYR	2.5
1	C	343	LYS	2.5
1	D	90	LEU	2.5
1	D	189	LEU	2.5
1	A	163	ILE	2.5
1	B	161	ASN	2.5
1	A	251	LEU	2.5
1	A	120	ALA	2.5
1	C	185	ARG	2.5
1	A	38	ARG	2.4
1	B	129	MET	2.4
1	C	348	LEU	2.4
1	C	39	ASN	2.4
1	D	282	TYR	2.4
1	B	262	ILE	2.4
1	C	366	LYS	2.4
1	B	159	LEU	2.4
1	C	362	GLU	2.4
1	D	93	GLU	2.4
1	A	191	THR	2.4
1	B	328	ILE	2.4
1	B	372	ALA	2.4
1	A	162	SER	2.4
1	C	160	TYR	2.4
1	C	228	ILE	2.4
1	C	247	TYR	2.4
1	B	197	LEU	2.4
1	D	125	ALA	2.4
1	D	204	ASP	2.3
1	D	181	ILE	2.3
1	A	247	TYR	2.3
1	D	61	ILE	2.3
1	D	289	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	311	LEU	2.3
1	C	118	LEU	2.3
1	C	123	LEU	2.3
1	B	243	LYS	2.3
1	A	161	ASN	2.3
1	A	340	ALA	2.3
1	D	35	ALA	2.3
1	B	371	SER	2.3
1	B	302	VAL	2.3
1	C	173	ASN	2.3
1	B	121	ALA	2.3
1	B	166	LEU	2.3
1	C	385	LEU	2.3
1	C	329	LYS	2.3
1	B	251	LEU	2.3
1	B	376	LEU	2.3
1	C	54	GLU	2.3
1	C	216	ASN	2.2
1	C	327	LYS	2.2
1	C	249	PHE	2.2
1	A	182	ALA	2.2
1	A	245	ALA	2.2
1	A	188	THR	2.2
1	B	240	VAL	2.2
1	C	211	ARG	2.2
1	B	128	ILE	2.2
1	C	251	LEU	2.2
1	D	286	HIS	2.2
1	D	60	GLU	2.2
1	B	114	CYS	2.2
1	B	184	PHE	2.2
1	C	224	PRO	2.2
1	C	246	TYR	2.2
1	D	340	ALA	2.2
1	C	100	ILE	2.2
1	C	191	THR	2.2
1	D	59	GLU	2.2
1	C	364	ALA	2.1
1	D	187	ALA	2.1
1	C	392	LEU	2.1
1	D	325	PRO	2.1
1	C	289	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	250	PHE	2.1
1	B	367	ALA	2.1
1	C	374	ASN	2.1
1	B	112	ALA	2.1
1	B	364	ALA	2.1
1	C	138	LYS	2.1
1	D	283	PHE	2.1
1	B	325	PRO	2.1
1	A	155	ASP	2.1
1	A	289	TYR	2.1
1	C	181	ILE	2.1
1	C	388	LEU	2.1
1	D	111	LEU	2.1
1	D	389	LEU	2.1
1	C	137	ASN	2.1
1	C	103	SER	2.1
1	C	282	TYR	2.1
1	B	255	CYS	2.1
1	C	156	VAL	2.1
1	C	286	HIS	2.0
1	C	292	ILE	2.0
1	C	257	MET	2.0
1	C	261	GLY	2.0
1	C	95	VAL	2.0
1	D	215	VAL	2.0
1	C	226	ILE	2.0
1	D	119	GLN	2.0
1	D	303	GLY	2.0
1	C	142	TYR	2.0
1	B	195	GLN	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 ⓘ

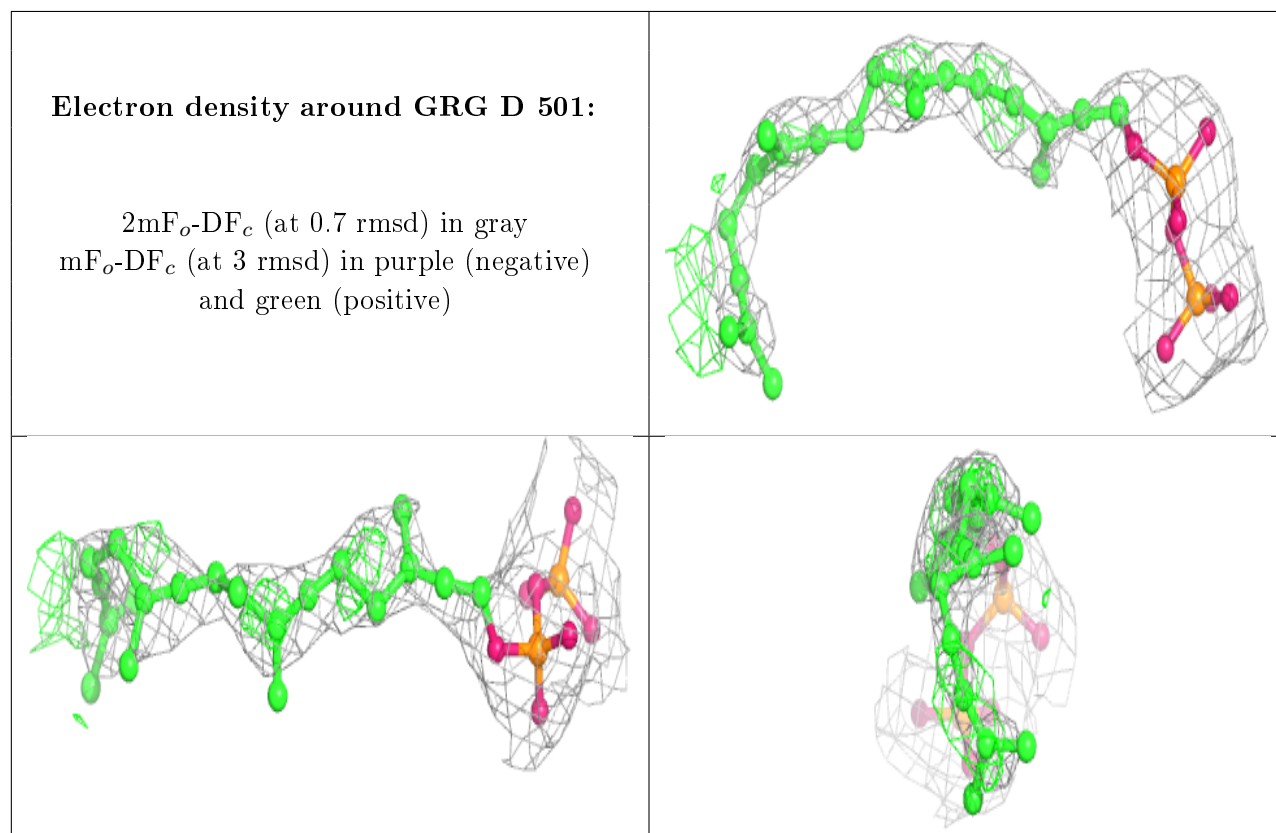
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

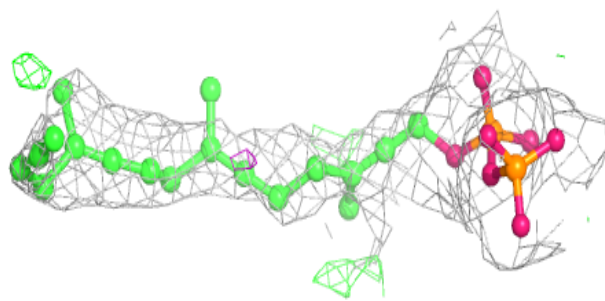
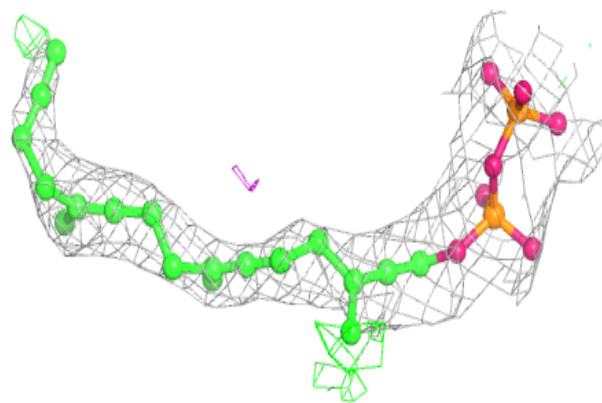
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GRG	D	501	29/29	0.93	0.37	38,49,65,65	20
3	GRG	C	501	27/29	0.94	0.21	67,70,74,75	0
2	NA	A	502	1/1	0.94	0.15	54,54,54,54	0
3	GRG	A	501	29/29	0.96	0.17	43,48,54,55	0
3	GRG	B	501	29/29	0.96	0.21	43,49,51,52	0

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.

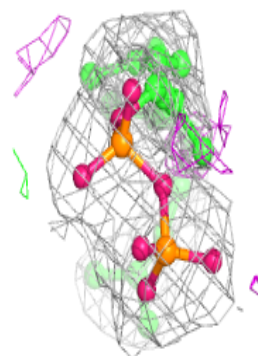
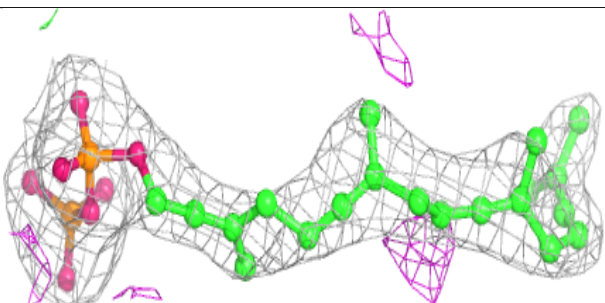
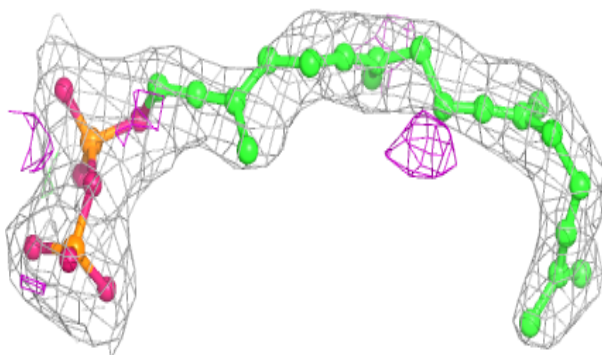


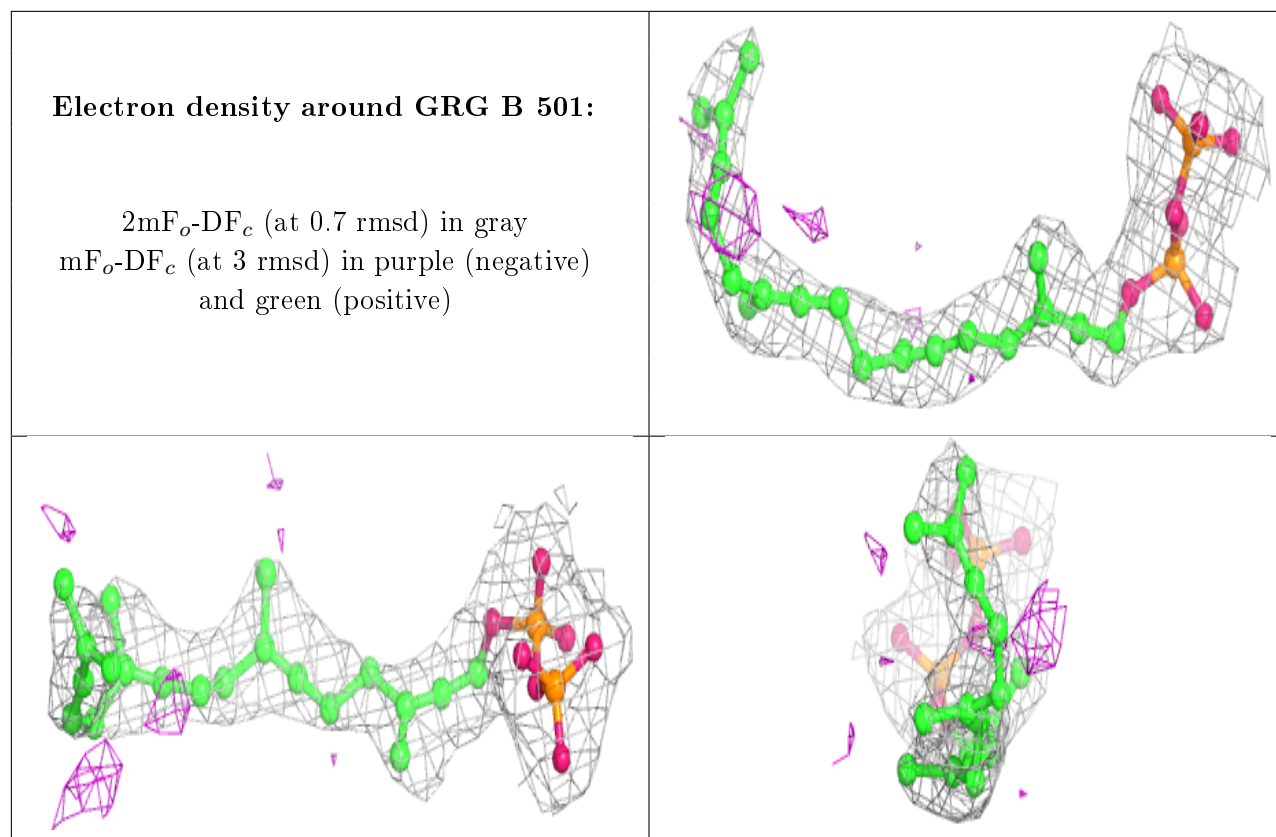
Electron density around GRG C 501:

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

**Electron density around GRG 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.