



## Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:19 PM UTC

PDB ID : 3PH7 / pdb\_00003ph7  
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.; Schapiro, M.; Bochkarev, A.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Hui, R.; Artz, J.D.; Structural Genomics Consortium (SGC)  
Deposited on : 2010-11-03  
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](mailto: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>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

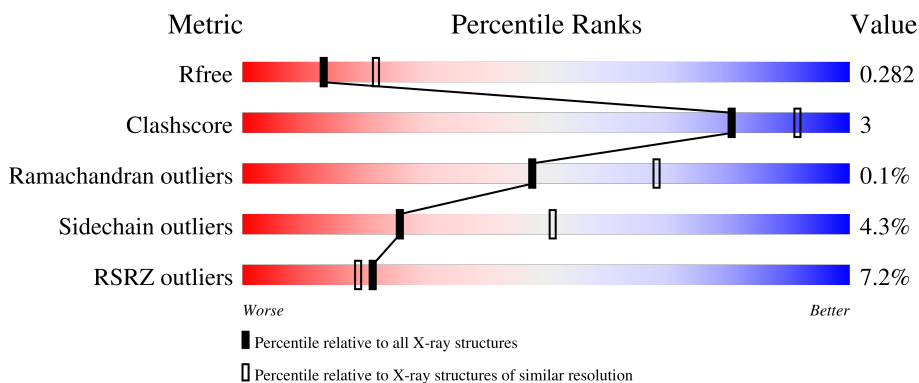
# 1 Overall quality at a glance i

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))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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  $\geq 3$ , 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	
1	B	396	
1	C	396	
1	D	396	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 10876 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 Farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	347	2757	1791	438	513	15	0	0	0
1	B	359	2875	1866	460	534	15	0	1	0
1	C	331	2462	1578	410	460	14	0	0	0
1	D	339	2576	1666	410	485	15	0	0	0

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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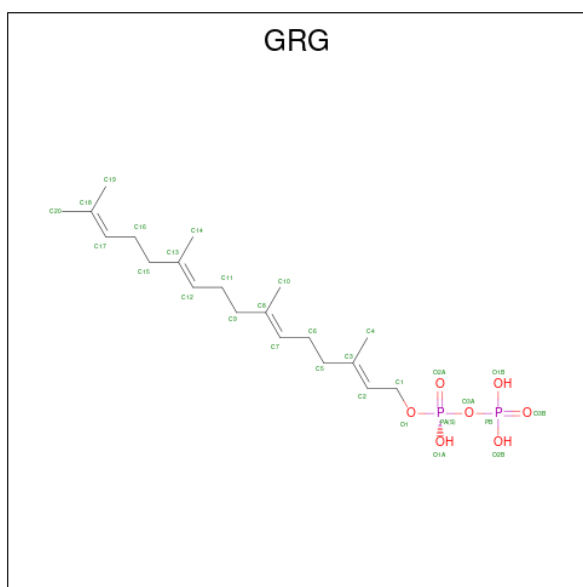
Chain	Residue	Modelled	Actual	Comment	Reference
A	134	MET	THR	conflict	UNP A5K4U6
A	227	ASP	ASN	conflict	UNP A5K4U6
B	1	MET	-	expression tag	UNP A5K4U6
B	2	GLY	-	expression tag	UNP A5K4U6
B	3	SER	-	expression tag	UNP A5K4U6
B	4	SER	-	expression tag	UNP A5K4U6
B	5	HIS	-	expression tag	UNP A5K4U6
B	6	HIS	-	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	conflict	UNP A5K4U6
B	227	ASP	ASN	conflict	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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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	conflict	UNP A5K4U6
C	227	ASP	ASN	conflict	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	conflict	UNP A5K4U6
D	227	ASP	ASN	conflict	UNP A5K4U6

- Molecule 2 is GERANYLGERANYL DIPHOSPHATE (CCD ID: GRG) (formula: C<sub>20</sub>H<sub>36</sub>O<sub>7</sub>P<sub>2</sub>).



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

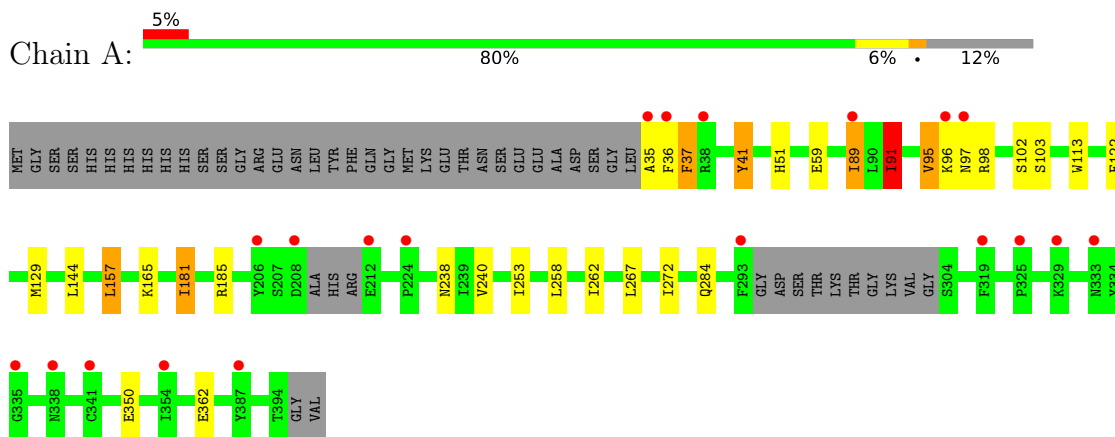
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	32	Total	O	0	0
			32	32		
3	C	10	Total	O	0	0
			10	10		
3	D	17	Total	O	0	0
			17	17		

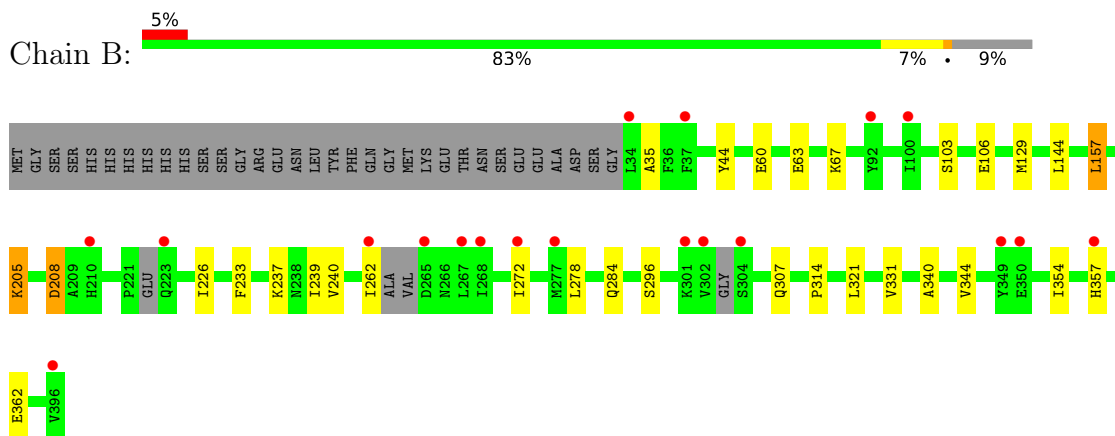
### 3 Residue-property plots [i](#)

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.

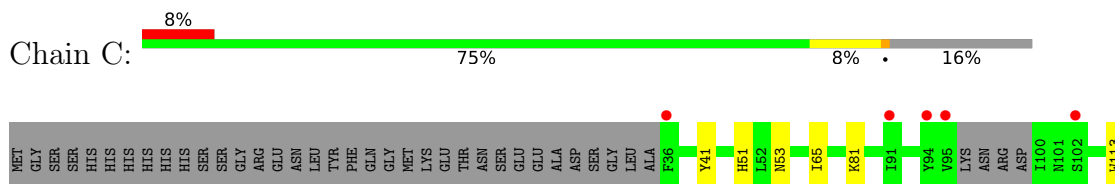
- Molecule 1: Farnesyl pyrophosphate synthase

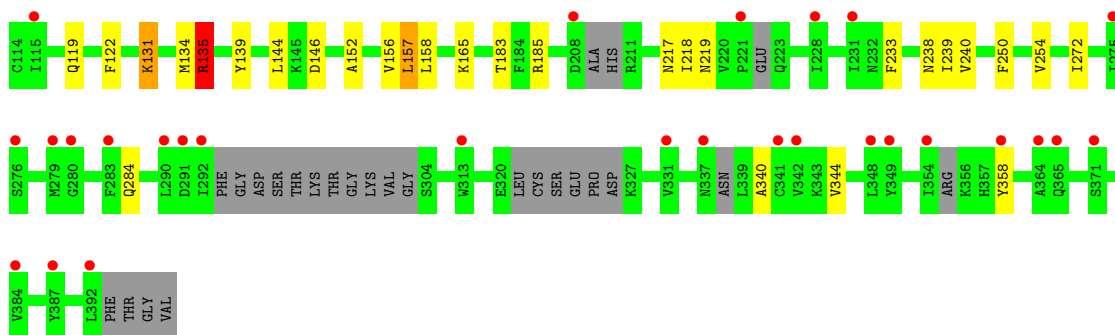


- Molecule 1: Farnesyl pyrophosphate synthase

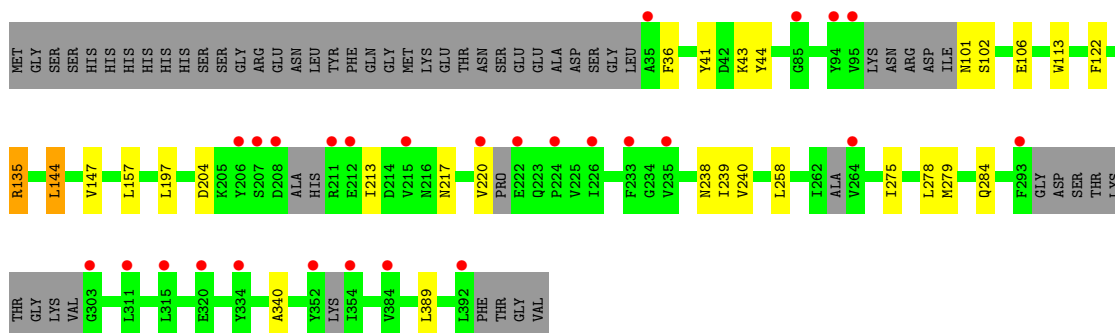
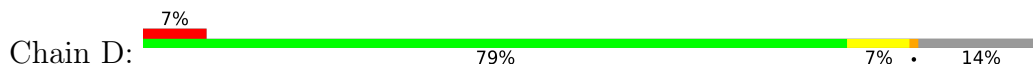


- Molecule 1: Farnesyl pyrophosphate synthase





- Molecule 1: Farnesyl pyrophosphate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.09Å 108.98Å 141.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.19 – 2.50 38.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.19-2.50) 99.7 (38.19-2.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.51Å)	Xtrriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.235 , 0.273 0.239 , 0.282	Depositor DCC
$R_{free}$ test set	2901 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.6	Xtrriage
Anisotropy	0.262	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.008 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.89	2/2816 (0.1%)	1.41	8/3828 (0.2%)
1	B	0.89	0/2938	1.40	4/3983 (0.1%)
1	C	0.85	0/2507	1.47	11/3417 (0.3%)
1	D	0.86	0/2625	1.43	11/3579 (0.3%)
All	All	0.87	2/10886 (0.0%)	1.43	34/14807 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	ILE	CG1-CD1	-7.98	1.20	1.51
1	A	89	ILE	CG1-CD1	-6.14	1.27	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	PHE	CA-C-N	7.51	130.67	120.38
1	A	36	PHE	C-N-CA	7.51	130.67	120.38
1	A	95	VAL	N-CA-C	-6.80	106.39	111.90
1	A	37	PHE	CA-CB-CG	6.62	120.42	113.80
1	B	208	ASP	CA-CB-CG	6.42	119.03	112.60
1	C	122	PHE	CA-C-N	6.29	129.04	120.54
1	C	122	PHE	C-N-CA	6.29	129.04	120.54
1	D	135	ARG	CA-CB-CG	-6.25	101.59	114.10
1	B	239	ILE	CA-C-N	6.24	129.01	120.46
1	B	239	ILE	C-N-CA	6.24	129.01	120.46
1	D	239	ILE	CA-C-N	6.21	128.96	120.46
1	D	239	ILE	C-N-CA	6.21	128.96	120.46
1	C	239	ILE	CA-C-N	6.12	128.85	120.46
1	C	239	ILE	C-N-CA	6.12	128.85	120.46
1	C	135	ARG	CA-CB-CG	-6.00	102.10	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	101	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	41	TYR	CA-C-N	5.70	128.19	120.38
1	A	41	TYR	C-N-CA	5.70	128.19	120.38
1	D	340	ALA	CA-C-N	5.62	127.80	120.28
1	D	340	ALA	C-N-CA	5.62	127.80	120.28
1	C	233	PHE	CA-CB-CG	5.53	119.33	113.80
1	D	144	LEU	CA-C-N	5.50	127.92	120.38
1	D	144	LEU	C-N-CA	5.50	127.92	120.38
1	A	238	ASN	CA-CB-CG	5.38	117.98	112.60
1	A	181	ILE	N-CA-CB	5.31	117.76	110.54
1	D	36	PHE	CA-C-N	5.23	127.24	120.44
1	D	36	PHE	C-N-CA	5.23	127.24	120.44
1	C	131	LYS	CA-C-N	5.13	126.03	120.44
1	C	131	LYS	C-N-CA	5.13	126.03	120.44
1	C	238	ASN	CA-CB-CG	5.12	117.72	112.60
1	B	35	ALA	N-CA-C	-5.10	105.80	111.36
1	C	358	TYR	CA-C-N	5.05	127.05	120.28
1	C	358	TYR	C-N-CA	5.05	127.05	120.28
1	D	238	ASN	CA-CB-CG	5.03	117.63	112.60

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	2757	0	2587	12	0
1	B	2875	0	2728	11	0
1	C	2462	0	2115	21	0
1	D	2576	0	2295	12	0
2	A	29	0	21	4	0
2	B	29	0	21	3	0
2	C	27	0	15	4	0
2	D	29	0	21	4	0
3	A	33	0	0	0	0
3	B	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	10	0	0	0	0
3	D	17	0	0	0	0
All	All	10876	0	9803	54	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 3.

All (54) 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:157:LEU:HD22	2:B:1502:GRG:H203	1.36	1.03
1:C:157:LEU:HD22	2:D:1502:GRG:H203	1.57	0.87
1:B:240:VAL:HG22	1:B:284:GLN:HG2	1.64	0.79
1:D:240:VAL:HG22	1:D:284:GLN:HG2	1.69	0.74
1:A:240:VAL:HG22	1:A:284:GLN:HG2	1.70	0.73
1:C:240:VAL:HG22	1:C:284:GLN:HG2	1.69	0.73
1:C:183:THR:HG21	1:C:254:VAL:HG23	1.76	0.66
1:A:157:LEU:HD22	2:B:1502:GRG:C20	2.20	0.65
1:C:183:THR:HG21	1:C:254:VAL:CG2	2.28	0.64
2:A:1502:GRG:H203	1:B:157:LEU:HD22	1.84	0.60
1:C:250:PHE:O	1:C:254:VAL:HG22	2.02	0.59
1:A:91:ILE:O	1:A:95:VAL:HG22	2.04	0.58
1:C:135:ARG:HH22	2:C:1502:GRG:HC43	1.68	0.58
1:C:51:HIS:CE1	1:C:165:LYS:HE2	2.39	0.56
1:C:65:ILE:HD11	1:D:197:LEU:HD21	1.87	0.56
1:A:129:MET:HE1	2:A:1502:GRG:H152	1.89	0.54
1:C:152:ALA:O	1:C:156:VAL:HG23	2.07	0.54
1:A:35:ALA:C	1:A:37:PHE:H	2.15	0.53
1:D:122:PHE:HE1	2:D:1502:GRG:H202	1.77	0.49
1:C:81:LYS:NZ	2:C:1502:GRG:O1A	2.43	0.49
1:B:321:LEU:HD21	1:B:357:HIS:NE2	2.27	0.49
1:C:217:ASN:OD1	1:C:219:ASN:HB3	2.12	0.48
1:C:134:MET:HE1	1:C:139:TYR:CE2	2.48	0.48
1:A:51:HIS:CE1	1:A:165:LYS:HE2	2.48	0.48
1:D:43:LYS:NZ	1:D:106:GLU:HG3	2.28	0.48
1:D:41:TYR:HB2	1:D:113:TRP:CZ2	2.50	0.47
1:B:129:MET:HE1	2:B:1502:GRG:H152	1.97	0.46
1:B:314:PRO:HB3	1:B:354:ILE:HG21	1.97	0.46
1:A:96:LYS:O	1:A:98:ARG:N	2.48	0.46
1:A:122:PHE:HE1	2:A:1502:GRG:H202	1.81	0.46
1:D:279:MET:HE3	1:D:389:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:MET:CE	2:A:1502:GRG:H152	2.46	0.45
1:B:340:ALA:O	1:B:344:VAL:HG23	2.16	0.45
1:C:146:ASP:HB2	1:D:213:ILE:HG23	1.97	0.45
1:B:226:ILE:HD11	1:B:331:VAL:HG22	1.98	0.45
1:D:217:ASN:HD21	1:D:220:VAL:HB	1.82	0.45
1:B:60:GLU:O	1:B:63:GLU:HG2	2.18	0.44
1:C:157:LEU:HD22	2:D:1502:GRG:C20	2.38	0.44
1:D:275:ILE:O	1:D:279:MET:HG3	2.17	0.44
1:C:135:ARG:NH2	2:C:1502:GRG:HC43	2.32	0.43
1:C:183:THR:CG2	1:C:254:VAL:HG21	2.48	0.43
1:C:41:TYR:HB2	1:C:113:TRP:CZ2	2.53	0.43
1:C:340:ALA:O	1:C:344:VAL:HG23	2.19	0.43
1:A:41:TYR:HB2	1:A:113:TRP:CZ2	2.54	0.43
1:C:119:GLN:HE22	2:C:1502:GRG:C1	2.31	0.42
1:B:233:PHE:CE2	1:B:237:LYS:HD2	2.54	0.42
1:D:43:LYS:HZ3	1:D:106:GLU:HG3	1.84	0.42
1:B:44:TYR:OH	1:B:106:GLU:O	2.34	0.41
1:B:205:LYS:H	1:B:205:LYS:HG3	1.72	0.41
1:C:183:THR:CG2	1:C:254:VAL:CG2	2.98	0.41
1:C:134:MET:HE1	1:C:139:TYR:CD2	2.56	0.41
1:A:91:ILE:HD13	1:A:253:ILE:HA	2.03	0.41
1:D:44:TYR:OH	1:D:106:GLU:O	2.36	0.40
1:D:122:PHE:CD1	2:D:1502:GRG:H193	2.56	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	341/396 (86%)	327 (96%)	13 (4%)	1 (0%)	36 55
1	B	352/396 (89%)	338 (96%)	14 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	315/396 (80%)	305 (97%)	10 (3%)	0	100	100
1	D	325/396 (82%)	311 (96%)	14 (4%)	0	100	100
All	All	1333/1584 (84%)	1281 (96%)	51 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ASN

### 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	275/357 (77%)	260 (94%)	15 (6%)	19	40
1	B	291/357 (82%)	279 (96%)	12 (4%)	27	53
1	C	211/357 (59%)	202 (96%)	9 (4%)	26	51
1	D	237/357 (66%)	229 (97%)	8 (3%)	32	60
All	All	1014/1428 (71%)	970 (96%)	44 (4%)	26	51

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	89	ILE
1	A	91	ILE
1	A	102	SER
1	A	103	SER
1	A	144	LEU
1	A	157	LEU
1	A	181	ILE
1	A	185	ARG
1	A	258	LEU
1	A	262	ILE

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Mol	Chain	Res	Type
1	A	267	LEU
1	A	272	ILE
1	A	350	GLU
1	A	362	GLU
1	B	67	LYS
1	B	103	SER
1	B	144	LEU
1	B	157	LEU
1	B	205	LYS
1	B	208	ASP
1	B	262	ILE
1	B	272	ILE
1	B	278	LEU
1	B	296	SER
1	B	307	GLN
1	B	362	GLU
1	C	53	ASN
1	C	131	LYS
1	C	135	ARG
1	C	144	LEU
1	C	157	LEU
1	C	158	LEU
1	C	185	ARG
1	C	218	ILE
1	C	272	ILE
1	D	102	SER
1	D	135	ARG
1	D	144	LEU
1	D	147	VAL
1	D	157	LEU
1	D	204	ASP
1	D	258	LEU
1	D	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	64	HIS
1	A	266	ASN
1	B	195	GLN
1	B	219	ASN

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Mol	Chain	Res	Type
1	B	309	ASN
1	C	82	ASN
1	C	266	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	GRG	D	1502	-	27,28,28	3.34	8 (29%)	33,37,37	8.28	9 (27%)
2	GRG	A	1502	-	27,28,28	3.25	8 (29%)	33,37,37	8.27	10 (30%)
2	GRG	B	1502	-	27,28,28	3.31	8 (29%)	33,37,37	8.11	10 (30%)
2	GRG	C	1502	-	25,26,28	3.26	8 (32%)	30,34,37	8.54	8 (26%)

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	GRG	D	1502	-	-	14/31/31/31	-
2	GRG	A	1502	-	-	12/31/31/31	-
2	GRG	B	1502	-	-	13/31/31/31	-
2	GRG	C	1502	-	-	14/29/29/31	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1502	GRG	C1-C2	-8.46	1.25	1.49
2	C	1502	GRG	C1-C2	-8.34	1.25	1.49
2	B	1502	GRG	C6-C7	-8.21	1.25	1.50
2	D	1502	GRG	C1-C2	-8.20	1.26	1.49
2	D	1502	GRG	C6-C7	-8.15	1.25	1.50
2	C	1502	GRG	C6-C7	-8.06	1.26	1.50
2	C	1502	GRG	C11-C12	-8.04	1.26	1.50
2	A	1502	GRG	C1-C2	-7.90	1.26	1.49
2	A	1502	GRG	C6-C7	-7.90	1.26	1.50
2	A	1502	GRG	C11-C12	-7.88	1.26	1.50
2	D	1502	GRG	C16-C17	-7.83	1.26	1.50
2	D	1502	GRG	C11-C12	-7.76	1.27	1.50
2	B	1502	GRG	C16-C17	-7.58	1.27	1.50
2	B	1502	GRG	C11-C12	-7.54	1.27	1.50
2	A	1502	GRG	C16-C17	-7.52	1.27	1.50
2	C	1502	GRG	C16-C17	-5.14	1.26	1.49
2	B	1502	GRG	C7-C8	-3.40	1.25	1.33
2	B	1502	GRG	C2-C3	-3.28	1.25	1.33
2	D	1502	GRG	C7-C8	-3.22	1.25	1.33
2	C	1502	GRG	C2-C3	-3.22	1.25	1.33
2	D	1502	GRG	PA-O3A	3.13	1.62	1.59
2	D	1502	GRG	C2-C3	-3.03	1.26	1.33
2	A	1502	GRG	PA-O3A	2.94	1.62	1.59
2	C	1502	GRG	C7-C8	-2.93	1.26	1.33
2	A	1502	GRG	C12-C13	-2.88	1.26	1.33
2	C	1502	GRG	C12-C13	-2.88	1.26	1.33
2	C	1502	GRG	PA-O3A	2.82	1.62	1.59
2	A	1502	GRG	C7-C8	-2.79	1.26	1.33
2	D	1502	GRG	C12-C13	-2.66	1.27	1.33
2	A	1502	GRG	C2-C3	-2.64	1.27	1.33
2	B	1502	GRG	PA-O3A	2.63	1.62	1.59
2	B	1502	GRG	C12-C13	-2.48	1.27	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1502	GRG	C1-C2-C3	32.46	179.39	126.20
2	A	1502	GRG	C1-C2-C3	32.33	179.17	126.20
2	D	1502	GRG	C1-C2-C3	32.03	178.67	126.20
2	B	1502	GRG	C1-C2-C3	31.18	177.29	126.20
2	C	1502	GRG	C6-C7-C8	22.65	179.47	127.62
2	D	1502	GRG	C6-C7-C8	22.35	178.79	127.62
2	C	1502	GRG	C11-C12-C13	22.28	178.63	127.62
2	B	1502	GRG	C11-C12-C13	22.15	178.32	127.62
2	A	1502	GRG	C6-C7-C8	21.62	177.11	127.62
2	A	1502	GRG	C11-C12-C13	21.53	176.91	127.62
2	D	1502	GRG	C11-C12-C13	21.28	176.34	127.62
2	B	1502	GRG	C6-C7-C8	20.94	175.56	127.62
2	D	1502	GRG	C16-C17-C18	14.79	176.94	127.64
2	A	1502	GRG	C16-C17-C18	14.78	176.92	127.64
2	B	1502	GRG	C16-C17-C18	13.86	173.84	127.64
2	C	1502	GRG	C16-C17-C18	7.26	179.62	126.65
2	B	1502	GRG	C4-C3-C5	4.12	122.38	115.23
2	C	1502	GRG	C4-C3-C5	3.77	121.77	115.23
2	B	1502	GRG	C15-C16-C17	3.62	129.94	112.02
2	D	1502	GRG	C4-C3-C5	3.48	121.26	115.23
2	A	1502	GRG	C4-C3-C5	3.36	121.06	115.23
2	D	1502	GRG	C10-C8-C9	3.29	120.94	115.23
2	A	1502	GRG	C15-C16-C17	3.25	128.10	112.02
2	B	1502	GRG	C10-C8-C9	3.16	120.72	115.23
2	C	1502	GRG	C10-C8-C9	3.03	120.48	115.23
2	C	1502	GRG	C14-C13-C15	2.90	120.26	115.23
2	D	1502	GRG	C14-C13-C15	2.76	120.01	115.23
2	B	1502	GRG	C10-C8-C7	-2.63	116.87	123.63
2	C	1502	GRG	C15-C16-C17	2.45	121.20	112.95
2	A	1502	GRG	C14-C13-C12	-2.40	117.46	123.63
2	D	1502	GRG	C15-C16-C17	2.39	123.84	112.02
2	A	1502	GRG	C10-C8-C7	-2.39	117.50	123.63
2	B	1502	GRG	C9-C11-C12	2.23	123.03	112.02
2	A	1502	GRG	C10-C8-C9	2.22	119.09	115.23
2	A	1502	GRG	C9-C11-C12	2.06	122.20	112.02
2	D	1502	GRG	C14-C13-C12	-2.04	118.38	123.63
2	B	1502	GRG	O1A-PA-O2A	2.00	121.77	112.44

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1502	GRG	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	1502	GRG	C1-C2-C3-C4
2	B	1502	GRG	C11-C12-C13-C14
2	B	1502	GRG	C11-C12-C13-C15
2	B	1502	GRG	C1-C2-C3-C5
2	B	1502	GRG	C1-C2-C3-C4
2	B	1502	GRG	O1-C1-C2-C3
2	C	1502	GRG	C11-C12-C13-C14
2	C	1502	GRG	C1-C2-C3-C4
2	C	1502	GRG	PA-O3A-PB-O1B
2	D	1502	GRG	C6-C7-C8-C9
2	D	1502	GRG	C6-C7-C8-C10
2	D	1502	GRG	C1-C2-C3-C5
2	D	1502	GRG	C1-C2-C3-C4
2	D	1502	GRG	O1-C1-C2-C3
2	B	1502	GRG	C16-C17-C18-C19
2	A	1502	GRG	C16-C17-C18-C19
2	A	1502	GRG	C4-C3-C5-C6
2	C	1502	GRG	C4-C3-C5-C6
2	C	1502	GRG	C2-C3-C5-C6
2	A	1502	GRG	C16-C17-C18-C20
2	B	1502	GRG	C6-C7-C8-C10
2	D	1502	GRG	C11-C12-C13-C14
2	B	1502	GRG	C6-C7-C8-C9
2	C	1502	GRG	C11-C12-C13-C15
2	D	1502	GRG	C11-C12-C13-C15
2	B	1502	GRG	C16-C17-C18-C20
2	D	1502	GRG	C16-C17-C18-C19
2	A	1502	GRG	C2-C3-C5-C6
2	D	1502	GRG	C2-C3-C5-C6
2	A	1502	GRG	C12-C11-C9-C8
2	B	1502	GRG	C12-C11-C9-C8
2	D	1502	GRG	C12-C11-C9-C8
2	D	1502	GRG	C3-C5-C6-C7
2	B	1502	GRG	C4-C3-C5-C6
2	D	1502	GRG	C4-C3-C5-C6
2	B	1502	GRG	C2-C3-C5-C6
2	D	1502	GRG	C16-C17-C18-C20
2	A	1502	GRG	C3-C5-C6-C7
2	C	1502	GRG	C12-C11-C9-C8
2	C	1502	GRG	C3-C5-C6-C7
2	A	1502	GRG	C13-C15-C16-C17
2	B	1502	GRG	C13-C15-C16-C17

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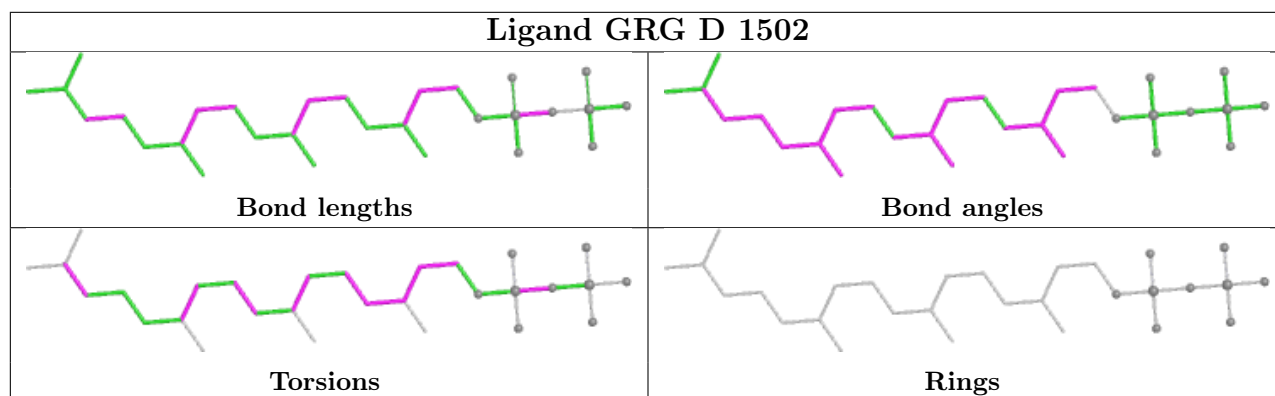
Mol	Chain	Res	Type	Atoms
2	C	1502	GRG	C6-C7-C8-C9
2	A	1502	GRG	C1-C2-C3-C5
2	C	1502	GRG	C6-C7-C8-C10
2	D	1502	GRG	PB-O3A-PA-O2A
2	A	1502	GRG	C9-C11-C12-C13
2	C	1502	GRG	C15-C16-C17-C18
2	C	1502	GRG	C1-C2-C3-C5
2	C	1502	GRG	PA-O3A-PB-O3B
2	C	1502	GRG	PA-O3A-PB-O2B
2	A	1502	GRG	PB-O3A-PA-O1A

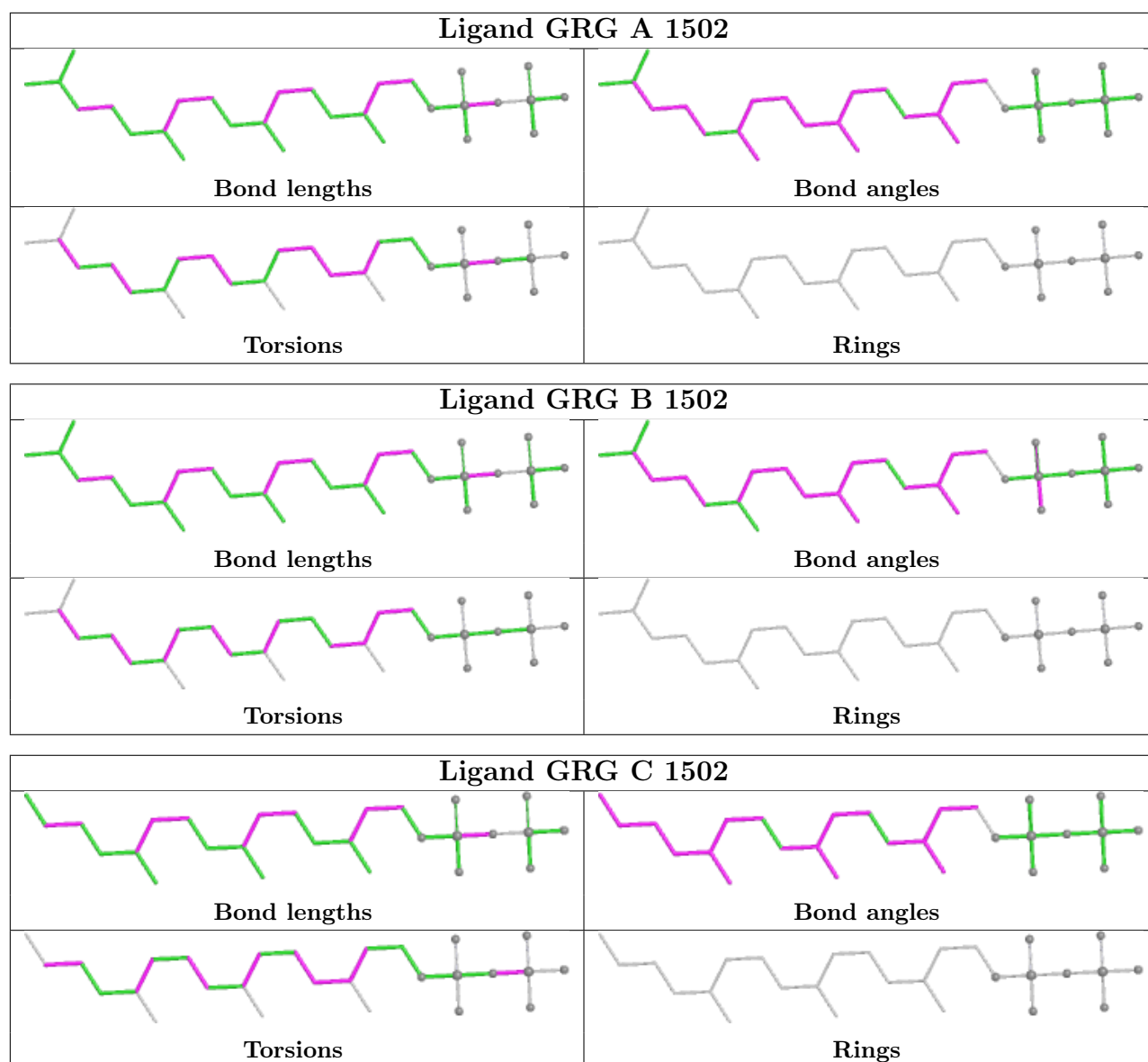
There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1502	GRG	4	0
2	A	1502	GRG	4	0
2	B	1502	GRG	3	0
2	C	1502	GRG	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	347/396 (87%)	0.43	20 (5%) 29 25	37, 60, 89, 114	11 (3%)
1	B	359/396 (90%)	0.39	19 (5%) 32 28	37, 60, 89, 123	5 (1%)
1	C	331/396 (83%)	0.87	33 (9%) 12 10	49, 83, 108, 131	2 (0%)
1	D	339/396 (85%)	0.73	27 (7%) 18 16	45, 70, 99, 121	0
All	All	1376/1584 (86%)	0.60	99 (7%) 21 19	37, 68, 102, 131	18 (1%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	302	VAL	6.8
1	D	208	ASP	6.3
1	C	283	PHE	5.5
1	C	208	ASP	5.4
1	A	208	ASP	5.1
1	B	396	VAL	4.1
1	D	94	TYR	3.9
1	B	265	ASP	3.8
1	D	220	VAL	3.5
1	D	334	TYR	3.5
1	C	290	LEU	3.4
1	D	222	GLU	3.4
1	C	292	ILE	3.4
1	C	392	LEU	3.3
1	C	291	ASP	3.3
1	C	276	SER	3.2
1	D	95	VAL	3.2
1	B	34	LEU	3.2
1	C	342	VAL	3.1
1	D	226	ILE	3.1
1	D	207	SER	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	354	ILE	3.0
1	D	354	ILE	3.0
1	C	91	ILE	3.0
1	C	280	GLY	3.0
1	D	392	LEU	2.9
1	B	350	GLU	2.9
1	D	293	PHE	2.9
1	A	341	CYS	2.9
1	C	95	VAL	2.8
1	A	38	ARG	2.8
1	C	387	TYR	2.8
1	D	212	GLU	2.8
1	D	303	GLY	2.8
1	C	279	MET	2.8
1	A	354	ILE	2.7
1	D	35	ALA	2.7
1	A	319	PHE	2.7
1	B	267	LEU	2.7
1	D	211	ARG	2.7
1	B	268	ILE	2.6
1	C	349	TYR	2.6
1	D	311	LEU	2.5
1	C	365	GLN	2.5
1	C	364	ALA	2.5
1	B	37	PHE	2.5
1	B	301	LYS	2.5
1	D	264	VAL	2.5
1	C	358	TYR	2.5
1	B	357	HIS	2.5
1	B	304	SER	2.5
1	C	102	SER	2.5
1	B	349	TYR	2.5
1	B	92	TYR	2.4
1	D	206	TYR	2.4
1	C	275	ILE	2.3
1	A	212	GLU	2.3
1	C	221	PRO	2.3
1	C	115	ILE	2.3
1	C	331	VAL	2.3
1	B	210	HIS	2.3
1	B	100	ILE	2.3
1	A	338	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	36	PHE	2.3
1	C	341	CYS	2.3
1	D	233	PHE	2.2
1	D	215	VAL	2.2
1	A	97	ASN	2.2
1	C	231	ILE	2.2
1	C	313	TRP	2.2
1	A	293	PHE	2.2
1	B	272	ILE	2.2
1	A	224	PRO	2.2
1	A	325	PRO	2.2
1	A	335	GLY	2.2
1	D	224	PRO	2.2
1	C	384	VAL	2.1
1	D	235	VAL	2.1
1	A	333	ASN	2.1
1	B	223	GLN	2.1
1	D	85	GLY	2.1
1	A	387	TYR	2.1
1	A	96	LYS	2.1
1	A	329	LYS	2.1
1	C	36	PHE	2.1
1	D	320	GLU	2.1
1	A	206	TYR	2.1
1	D	352	TYR	2.1
1	A	35	ALA	2.1
1	D	315	LEU	2.1
1	B	262	ILE	2.1
1	C	94	TYR	2.1
1	C	337	ASN	2.0
1	A	89	ILE	2.0
1	B	277	MET	2.0
1	D	384	VAL	2.0
1	C	348	LEU	2.0
1	C	228	ILE	2.0
1	C	371	SER	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](#)

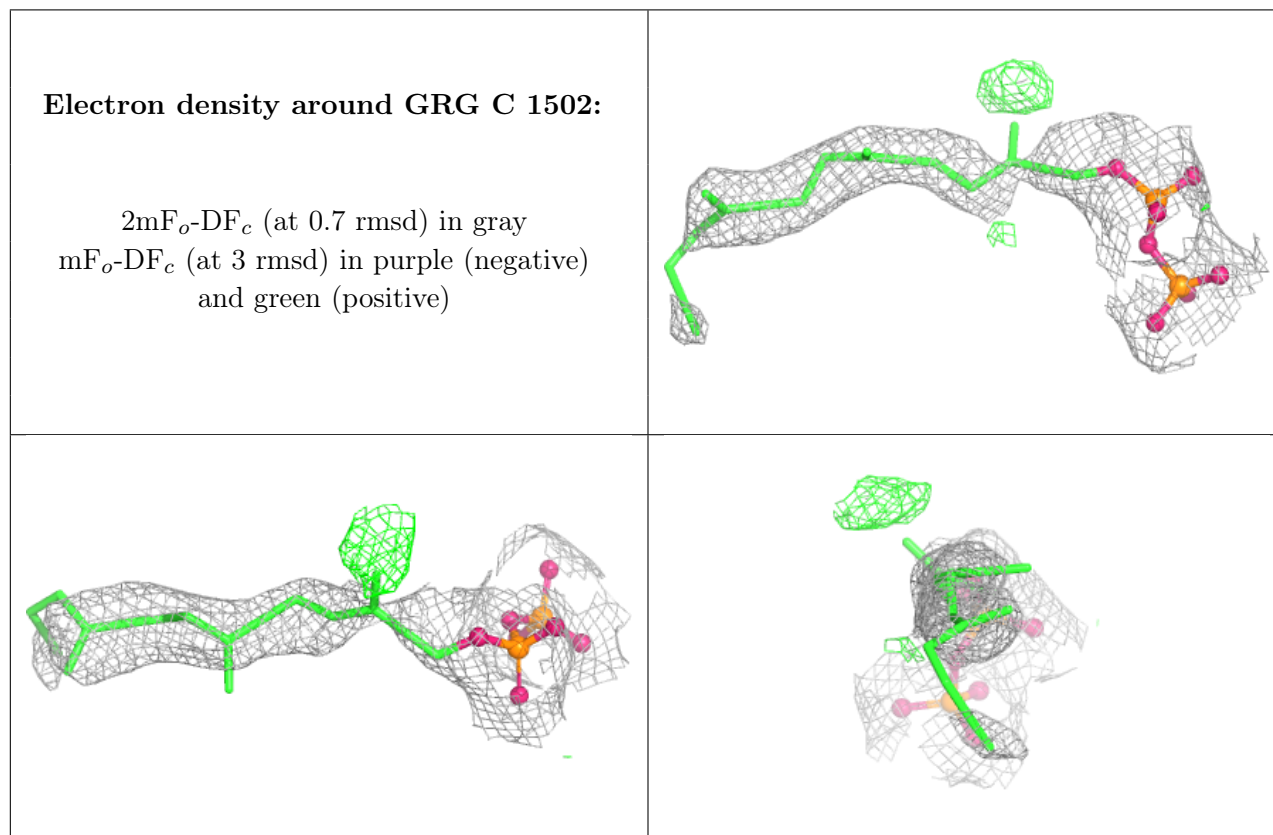
There are no oligosaccharides in this entry.

### 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, 95<sup>th</sup> 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.

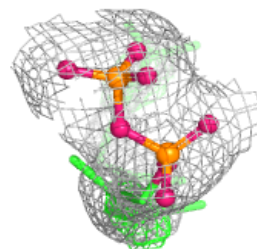
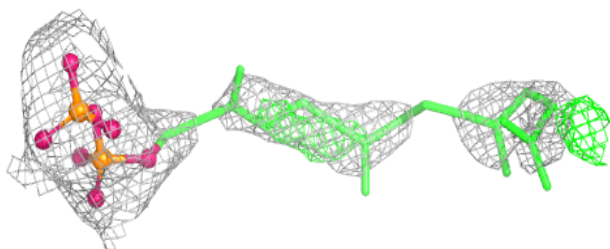
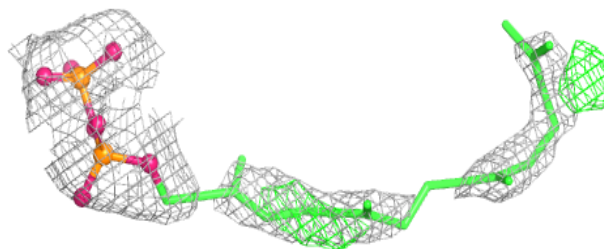
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GRG	C	1502	27/29	0.90	0.16	50,70,156,172	0
2	GRG	D	1502	29/29	0.93	0.17	23,49,95,169	20
2	GRG	B	1502	29/29	0.96	0.10	32,54,71,88	0
2	GRG	A	1502	29/29	0.97	0.09	34,52,84,95	0

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.

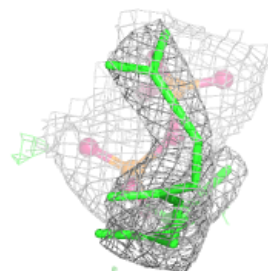
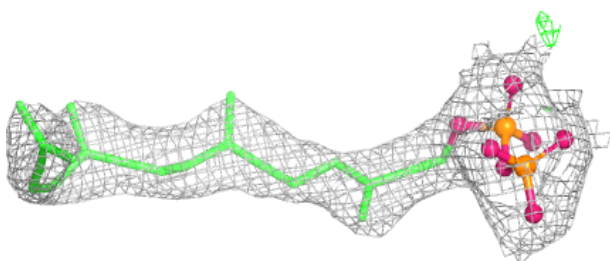
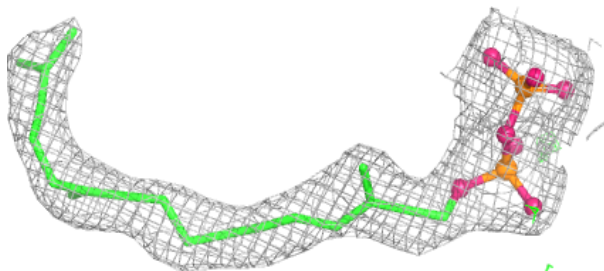


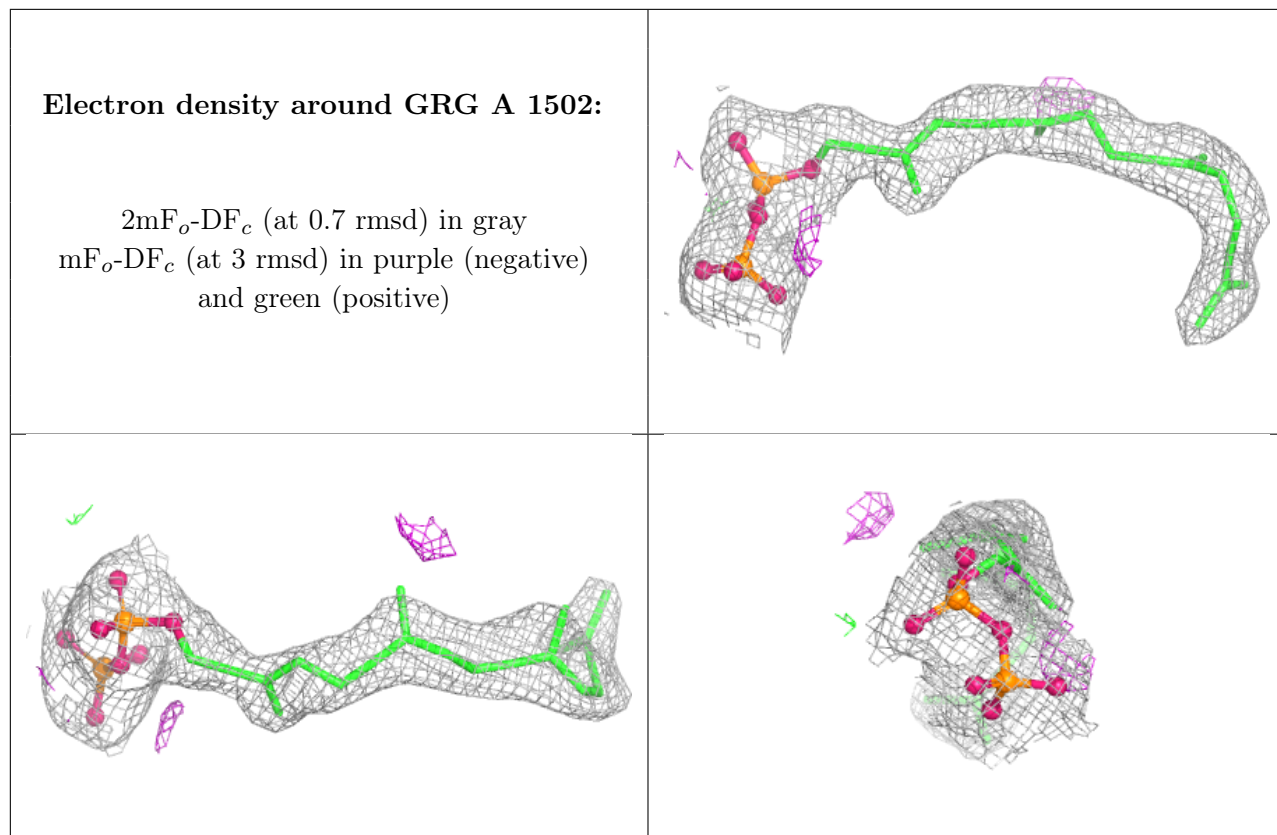
**Electron density around GRG D 1502:**

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

**Electron density around GRG B 1502:**

$2mF_o-DF_c$  (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.