Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 07:32 AM EST

PDB ID	:	3PH7
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.; Kozieradzki, 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

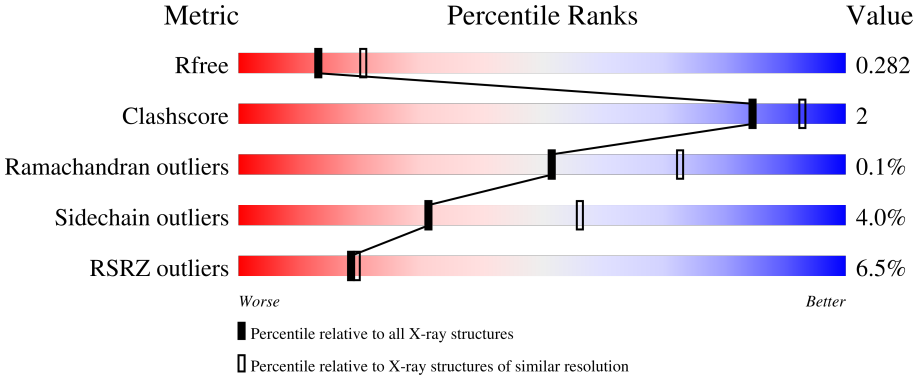
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	5% 81% 7% 12%
1	B	396	2% 84% 6% • 9%
1	C	396	9% 77% 6% 16%
1	D	396	7% 80% 6% 14%

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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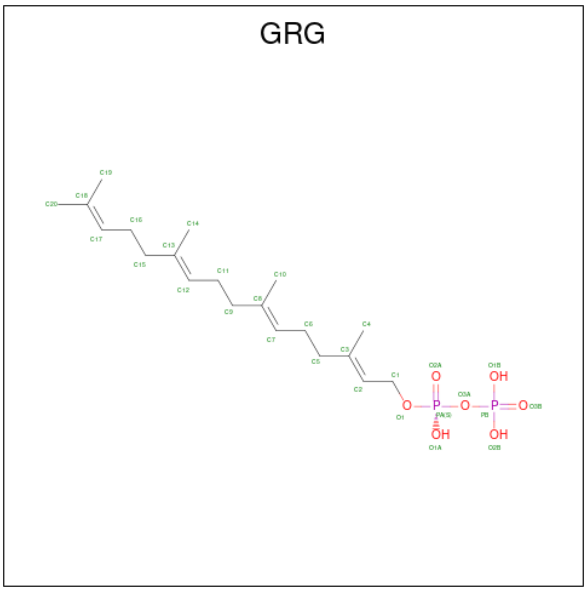
Chain	Residue	Modelled	Actual	Comment	Reference
C	18	TYR	-	expression tag	UNP A5K4U6
C	19	PHE	-	expression tag	UNP A5K4U6
C	20	GLN	-	expression tag	UNP A5K4U6
C	21	GLY	-	expression tag	UNP A5K4U6
C	134	MET	THR	conflict	UNP A5K4U6
C	227	ASP	ASN	conflict	UNP A5K4U6
D	1	MET	-	expression tag	UNP A5K4U6
D	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 (three-letter code: GRG) (formula: $C_{20}H_{36}O_7P_2$).



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

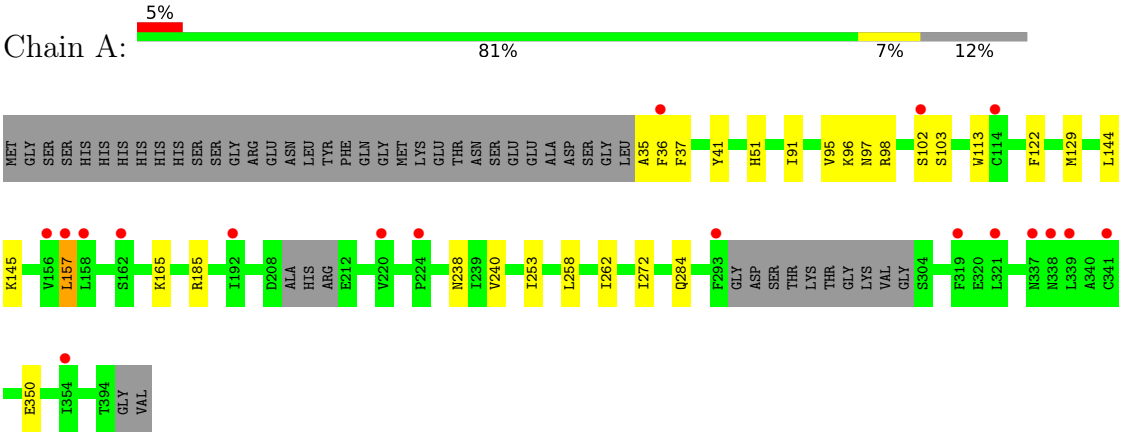
- Molecule 3 is water.

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

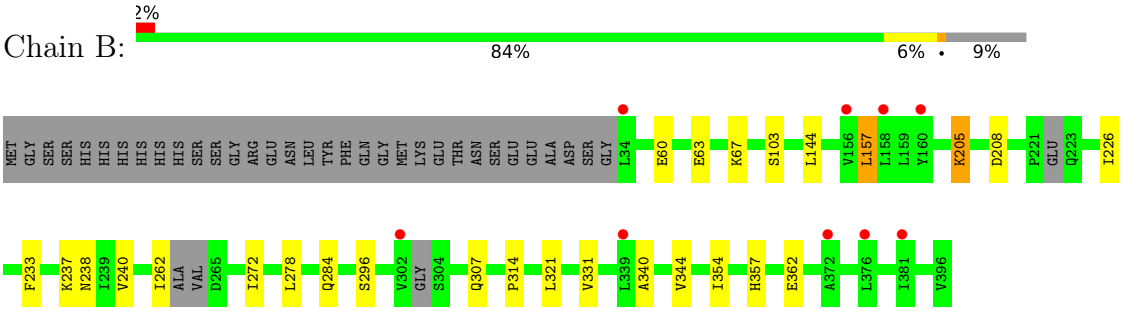
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

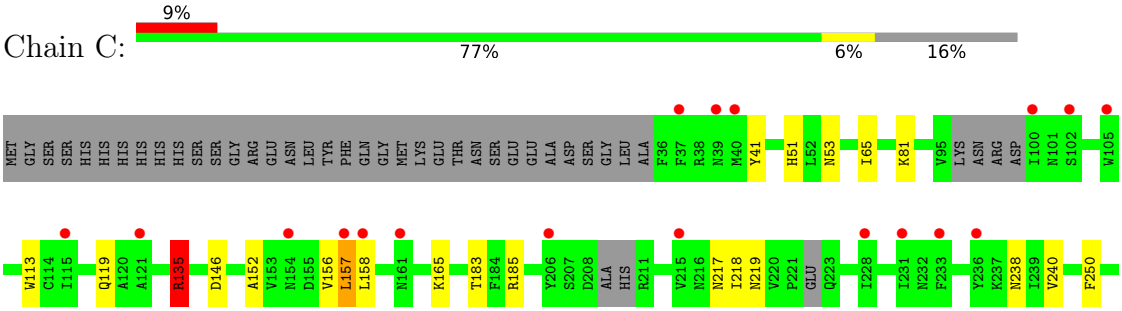
• Molecule 1: Farnesyl pyrophosphate synthase

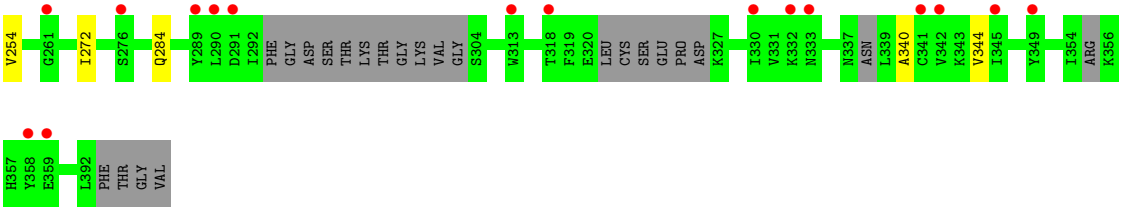


• Molecule 1: Farnesyl pyrophosphate synthase



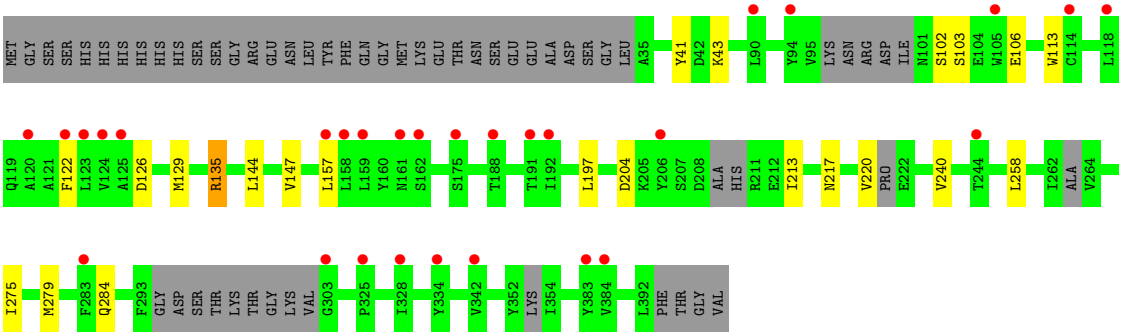
• Molecule 1: Farnesyl pyrophosphate synthase





- Molecule 1: Farnesyl pyrophosphate synthase

Chain D:



4 Data and refinement statistics (i)

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)	38.19 – 2.50 36.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.19-2.50) 99.8 (36.87-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.51Å)	Xtriage
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^2)	58.6	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10876	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage'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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.52	0/2816	0.65	0/3828
1	B	0.52	0/2938	0.67	0/3983
1	C	0.49	0/2507	0.64	1/3417 (0.0%)
1	D	0.49	0/2625	0.64	1/3579 (0.0%)
All	All	0.51	0/10886	0.65	2/14807 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	135	ARG	CA-CB-CG	-5.37	101.59	113.40
1	C	135	ARG	CA-CB-CG	-5.14	102.10	113.40

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	11	0
1	B	2875	0	2728	9	0
1	C	2462	0	2115	19	0
1	D	2576	0	2295	10	0
2	A	29	0	21	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	29	0	21	2	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
3	C	10	0	0	0	0
3	D	17	0	0	0	0
All	All	10876	0	9803	47	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 2.

All (47) 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:C:152:ALA:O	1:C:156:VAL:HG23	2.07	0.54
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:A:35:ALA:C	1:A:37:PHE:H	2.15	0.48
1:C:217:ASN:OD1	1:C:219:ASN:HB3	2.12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PHE:HE1	2:A:1502:GRG:H202	1.81	0.46
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: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:A:91:ILE:HD13	1:A:253:ILE:HA	2.03	0.41
1:D:122:PHE:CD1	2:D:1502:GRG:H193	2.56	0.40
1:D:126:ASP:HA	1:D:129:MET:HE3	2.04	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%)	41 61
1	B	352/396 (89%)	338 (96%)	14 (4%)	0	100 100
1	C	315/396 (80%)	305 (97%)	10 (3%)	0	100 100
1	D	325/396 (82%)	311 (96%)	14 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1333/1584 (84%)	1281 (96%)	51 (4%)	1 (0%)	51 73

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%)	263 (96%)	12 (4%)	28 52
1	B	291/357 (82%)	278 (96%)	13 (4%)	27 51
1	C	211/357 (59%)	203 (96%)	8 (4%)	33 58
1	D	237/357 (66%)	229 (97%)	8 (3%)	37 63
All	All	1014/1428 (71%)	973 (96%)	41 (4%)	31 56

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	PHE
1	A	102	SER
1	A	103	SER
1	A	144	LEU
1	A	145	LYS
1	A	157	LEU
1	A	185	ARG
1	A	238	ASN
1	A	258	LEU
1	A	262	ILE
1	A	272	ILE
1	A	350	GLU
1	B	67	LYS
1	B	103	SER

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Mol	Chain	Res	Type
1	B	144	LEU
1	B	157	LEU
1	B	205	LYS
1	B	208	ASP
1	B	238	ASN
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	135	ARG
1	C	157	LEU
1	C	158	LEU
1	C	185	ARG
1	C	218	ILE
1	C	238	ASN
1	C	272	ILE
1	D	102	SER
1	D	103	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

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	195	GLN
1	B	219	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 monosaccharides 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	-	26,28,28	3.13	8 (30%)	33,37,37	7.95	13 (39%)
2	GRG	B	1502	-	26,28,28	3.12	7 (26%)	33,37,37	7.80	10 (30%)
2	GRG	C	1502	-	24,26,28	3.11	7 (29%)	30,34,37	8.20	13 (43%)
2	GRG	A	1502	-	26,28,28	3.05	7 (26%)	33,37,37	7.94	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
2	GRG	D	1502	-	-	14/31/31/31	-
2	GRG	B	1502	-	-	13/31/31/31	-
2	GRG	C	1502	-	-	14/29/29/31	-
2	GRG	A	1502	-	-	11/31/31/31	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1502	GRG	C1-C2	-7.98	1.25	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1502	GRG	C1-C2	-7.88	1.25	1.49
2	D	1502	GRG	C1-C2	-7.75	1.26	1.49
2	B	1502	GRG	C6-C7	-7.61	1.25	1.50
2	D	1502	GRG	C6-C7	-7.56	1.25	1.50
2	C	1502	GRG	C6-C7	-7.47	1.26	1.50
2	A	1502	GRG	C1-C2	-7.46	1.26	1.49
2	C	1502	GRG	C11-C12	-7.45	1.26	1.50
2	A	1502	GRG	C6-C7	-7.32	1.26	1.50
2	A	1502	GRG	C11-C12	-7.30	1.26	1.50
2	D	1502	GRG	C16-C17	-7.25	1.26	1.50
2	D	1502	GRG	C11-C12	-7.19	1.27	1.50
2	B	1502	GRG	C16-C17	-7.02	1.27	1.50
2	B	1502	GRG	C11-C12	-6.98	1.27	1.50
2	A	1502	GRG	C16-C17	-6.97	1.27	1.50
2	C	1502	GRG	C16-C17	-5.33	1.26	1.49
2	B	1502	GRG	C7-C8	-3.23	1.25	1.33
2	B	1502	GRG	C2-C3	-3.12	1.25	1.33
2	D	1502	GRG	C7-C8	-3.06	1.25	1.33
2	C	1502	GRG	C2-C3	-3.05	1.25	1.33
2	D	1502	GRG	C2-C3	-2.87	1.26	1.33
2	C	1502	GRG	C7-C8	-2.78	1.26	1.33
2	A	1502	GRG	C12-C13	-2.73	1.26	1.33
2	C	1502	GRG	C12-C13	-2.73	1.26	1.33
2	A	1502	GRG	C7-C8	-2.64	1.26	1.33
2	D	1502	GRG	C12-C13	-2.51	1.27	1.33
2	A	1502	GRG	C2-C3	-2.50	1.27	1.33
2	B	1502	GRG	C12-C13	-2.35	1.27	1.33
2	D	1502	GRG	C17-C18	-2.00	1.26	1.32

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1502	GRG	C1-C2-C3	30.84	179.39	126.04
2	A	1502	GRG	C1-C2-C3	30.72	179.17	126.04
2	D	1502	GRG	C1-C2-C3	30.43	178.67	126.04
2	B	1502	GRG	C1-C2-C3	29.63	177.29	126.04
2	C	1502	GRG	C6-C7-C8	21.52	179.47	127.66
2	D	1502	GRG	C6-C7-C8	21.23	178.79	127.66
2	C	1502	GRG	C11-C12-C13	21.17	178.63	127.66
2	B	1502	GRG	C11-C12-C13	21.04	178.32	127.66
2	A	1502	GRG	C6-C7-C8	20.54	177.11	127.66
2	A	1502	GRG	C11-C12-C13	20.46	176.91	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1502	GRG	C11-C12-C13	20.22	176.34	127.66
2	B	1502	GRG	C6-C7-C8	19.89	175.56	127.66
2	D	1502	GRG	C16-C17-C18	14.39	176.94	127.75
2	A	1502	GRG	C16-C17-C18	14.39	176.92	127.75
2	B	1502	GRG	C16-C17-C18	13.49	173.84	127.75
2	C	1502	GRG	C16-C17-C18	7.76	179.62	126.84
2	B	1502	GRG	C15-C16-C17	5.49	129.94	111.88
2	A	1502	GRG	C15-C16-C17	4.93	128.10	111.88
2	B	1502	GRG	C4-C3-C5	4.23	122.38	115.27
2	C	1502	GRG	C4-C3-C5	3.86	121.77	115.27
2	D	1502	GRG	C15-C16-C17	3.64	123.84	111.88
2	D	1502	GRG	C4-C3-C5	3.56	121.26	115.27
2	A	1502	GRG	C4-C3-C5	3.44	121.06	115.27
2	B	1502	GRG	C9-C11-C12	3.39	123.03	111.88
2	D	1502	GRG	C10-C8-C9	3.37	120.94	115.27
2	C	1502	GRG	C15-C16-C17	3.33	121.20	112.63
2	B	1502	GRG	C10-C8-C9	3.24	120.72	115.27
2	A	1502	GRG	C9-C11-C12	3.14	122.20	111.88
2	C	1502	GRG	C10-C8-C9	3.10	120.48	115.27
2	C	1502	GRG	C9-C11-C12	3.03	121.83	111.88
2	C	1502	GRG	C5-C6-C7	3.03	121.83	111.88
2	C	1502	GRG	C14-C13-C15	2.97	120.26	115.27
2	D	1502	GRG	C9-C11-C12	2.93	121.52	111.88
2	D	1502	GRG	C14-C13-C15	2.82	120.01	115.27
2	B	1502	GRG	C10-C8-C7	-2.65	116.87	123.68
2	D	1502	GRG	PA-O3A-PB	-2.48	124.31	132.83
2	A	1502	GRG	C14-C13-C12	-2.42	117.46	123.68
2	A	1502	GRG	C10-C8-C7	-2.41	117.50	123.68
2	D	1502	GRG	C5-C6-C7	2.35	119.59	111.88
2	A	1502	GRG	O1-C1-C2	2.34	119.42	109.59
2	A	1502	GRG	C5-C6-C7	2.28	119.37	111.88
2	A	1502	GRG	C10-C8-C9	2.27	119.09	115.27
2	B	1502	GRG	C5-C6-C7	2.25	119.27	111.88
2	C	1502	GRG	O1-C1-C2	2.16	118.64	109.59
2	C	1502	GRG	PA-O3A-PB	-2.13	125.51	132.83
2	D	1502	GRG	C14-C13-C12	-2.06	118.38	123.68
2	C	1502	GRG	C4-C3-C2	-2.02	118.51	123.68
2	D	1502	GRG	O1-C1-C2	2.01	118.04	109.59

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1502	GRG	C5-C6-C7-C8
2	A	1502	GRG	C4-C3-C5-C6
2	A	1502	GRG	C1-C2-C3-C4
2	B	1502	GRG	C16-C17-C18-C19
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	C4-C3-C5-C6
2	C	1502	GRG	C2-C3-C5-C6
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	A	1502	GRG	C16-C17-C18-C19
2	A	1502	GRG	C16-C17-C18-C20
2	A	1502	GRG	C2-C3-C5-C6
2	C	1502	GRG	C1-C2-C3-C5
2	B	1502	GRG	C16-C17-C18-C20
2	D	1502	GRG	C16-C17-C18-C19
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	C4-C3-C5-C6
2	D	1502	GRG	C4-C3-C5-C6
2	B	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	A	1502	GRG	C1-C2-C3-C5
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

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Mol	Chain	Res	Type	Atoms
2	A	1502	GRG	C13-C15-C16-C17
2	B	1502	GRG	C13-C15-C16-C17
2	C	1502	GRG	C6-C7-C8-C9
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	PA-O3A-PB-O3B
2	C	1502	GRG	PA-O3A-PB-O2B

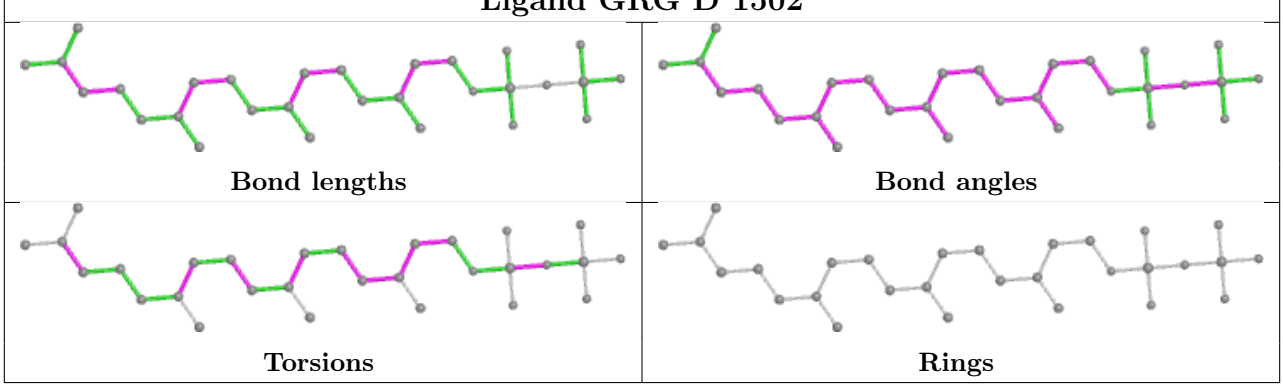
There are no ring outliers.

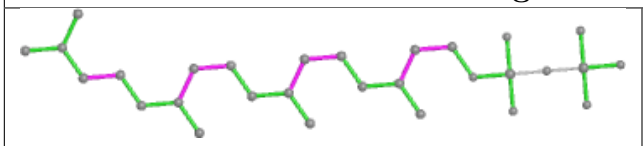
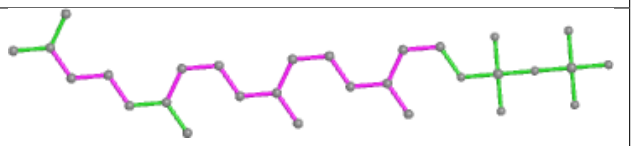
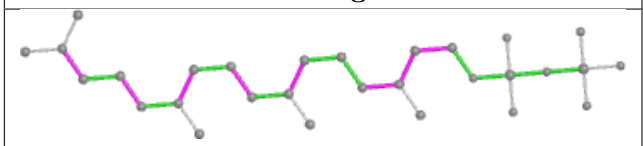
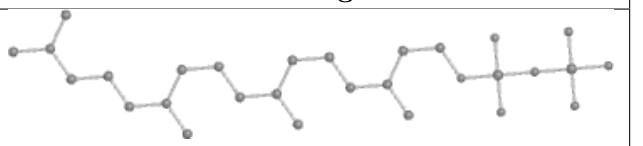
4 monomers are involved in 13 short contacts:

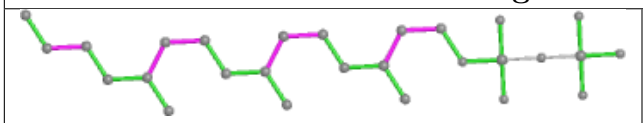
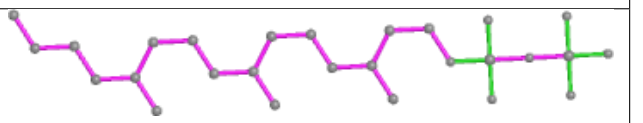
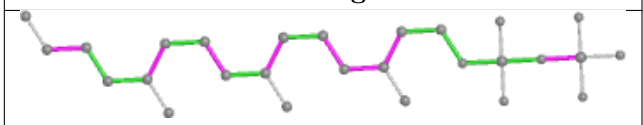
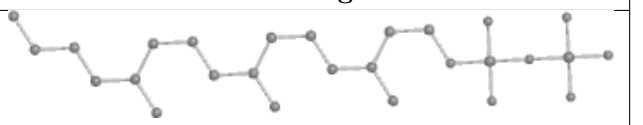
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1502	GRG	4	0
2	B	1502	GRG	2	0
2	C	1502	GRG	4	0
2	A	1502	GRG	3	0

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

Ligand GRG D 1502



Ligand GRG B 1502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GRG C 1502	
 Bond lengths	 Bond angles
 Torsions	 Rings

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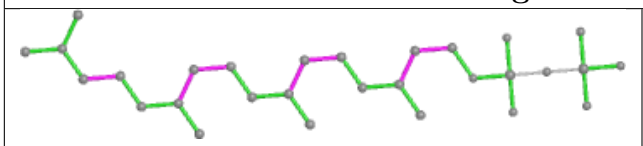
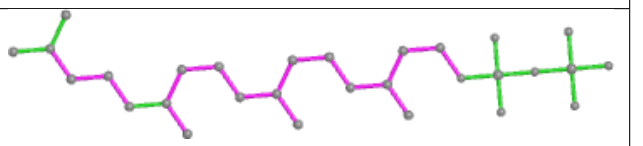
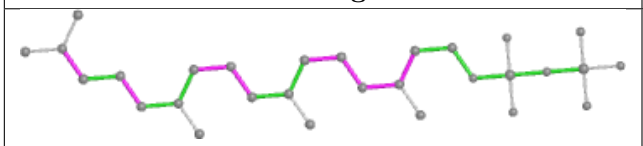
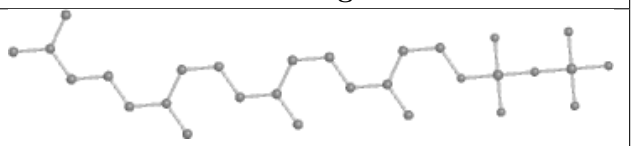
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	347/396 (87%)	0.12	18 (5%)	27	29	37, 60, 89, 114	11 (3%)
1	B	359/396 (90%)	0.16	9 (2%)	57	61	38, 60, 89, 123	4 (1%)
1	C	331/396 (83%)	0.66	34 (10%)	6	6	49, 83, 108, 131	2 (0%)
1	D	339/396 (85%)	0.36	29 (8%)	10	10	45, 70, 99, 121	0
All	All	1376/1584 (86%)	0.32	90 (6%)	18	19	37, 68, 102, 131	17 (1%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	TYR	5.3
1	C	341	CYS	5.2
1	C	359	GLU	4.8
1	C	291	ASP	4.7
1	C	102	SER	4.7
1	C	358	TYR	4.5
1	C	290	LEU	4.5
1	C	330	ILE	4.0
1	D	334	TYR	3.8
1	C	313	TRP	3.8
1	D	94	TYR	3.7
1	A	338	ASN	3.7
1	D	191	THR	3.6
1	A	341	CYS	3.6
1	B	34	LEU	3.5
1	D	192	ILE	3.4
1	C	345	ILE	3.3
1	C	100	ILE	3.3
1	C	342	VAL	3.2
1	C	233	PHE	3.2
1	C	40	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	158	LEU	3.1
1	D	188	THR	3.1
1	C	333	ASN	3.1
1	D	159	LEU	3.1
1	A	158	LEU	3.0
1	A	36	PHE	2.8
1	C	39	ASN	2.8
1	D	162	SER	2.8
1	C	276	SER	2.8
1	A	220	VAL	2.7
1	C	206	TYR	2.7
1	C	289	TYR	2.7
1	B	339	LEU	2.7
1	C	157	LEU	2.7
1	C	37	PHE	2.6
1	D	123	LEU	2.6
1	C	236	TYR	2.6
1	B	302	VAL	2.6
1	C	318	THR	2.6
1	D	325	PRO	2.6
1	A	319	PHE	2.5
1	C	231	ILE	2.5
1	C	105	TRP	2.5
1	C	121	ALA	2.5
1	C	228	ILE	2.5
1	B	158	LEU	2.5
1	B	372	ALA	2.5
1	B	376	LEU	2.5
1	A	224	PRO	2.5
1	D	125	ALA	2.5
1	C	161	ASN	2.5
1	D	384	VAL	2.4
1	D	161	ASN	2.4
1	A	192	ILE	2.4
1	D	206	TYR	2.3
1	C	261	GLY	2.3
1	D	90	LEU	2.3
1	D	124	VAL	2.3
1	A	156	VAL	2.3
1	D	342	VAL	2.3
1	D	283	PHE	2.2
1	A	321	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	158	LEU	2.2
1	C	332	LYS	2.2
1	D	114	CYS	2.2
1	A	354	ILE	2.2
1	A	293	PHE	2.2
1	A	102	SER	2.2
1	A	339	LEU	2.2
1	B	381	ILE	2.2
1	C	154	ASN	2.2
1	D	175	SER	2.2
1	D	118	LEU	2.2
1	A	162	SER	2.1
1	A	157	LEU	2.1
1	D	244	THR	2.1
1	B	160	TYR	2.1
1	D	122	PHE	2.1
1	D	303	GLY	2.1
1	D	157	LEU	2.1
1	A	337	ASN	2.1
1	D	120	ALA	2.1
1	D	328	ILE	2.1
1	D	383	TYR	2.0
1	D	105	TRP	2.0
1	C	215	VAL	2.0
1	A	114	CYS	2.0
1	B	156	VAL	2.0
1	C	115	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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,

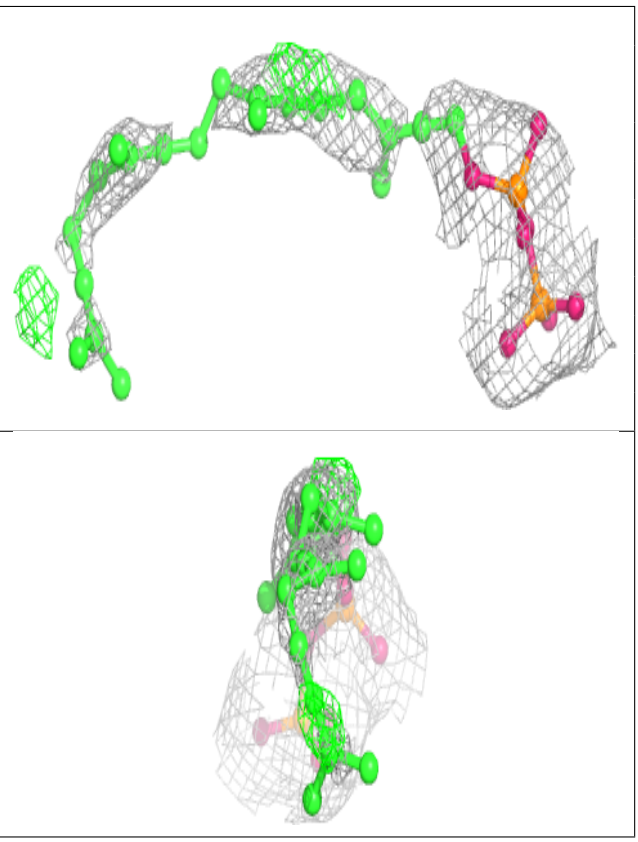
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GRG	D	1502	29/29	0.95	0.29	23,49,95,169	20
2	GRG	C	1502	27/29	0.96	0.20	50,70,156,172	0
2	GRG	A	1502	29/29	0.98	0.19	34,52,84,95	0
2	GRG	B	1502	29/29	0.98	0.20	32,54,71,88	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.

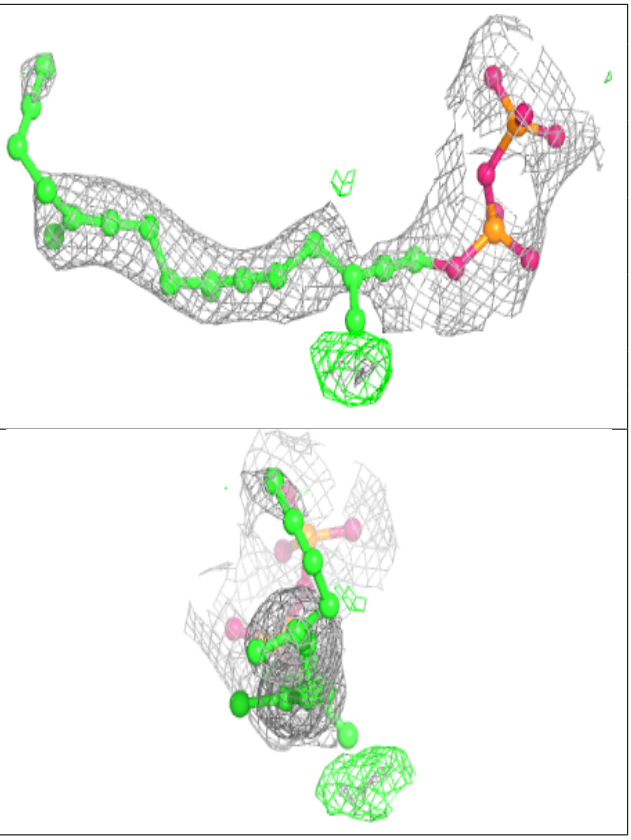
Electron density around GRG D 1502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



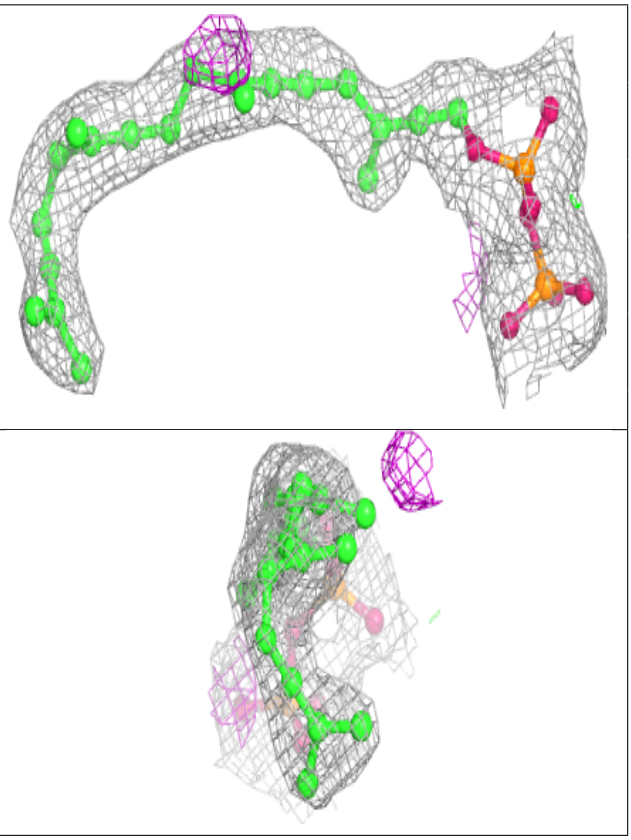
Electron density around GRG C 1502:

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



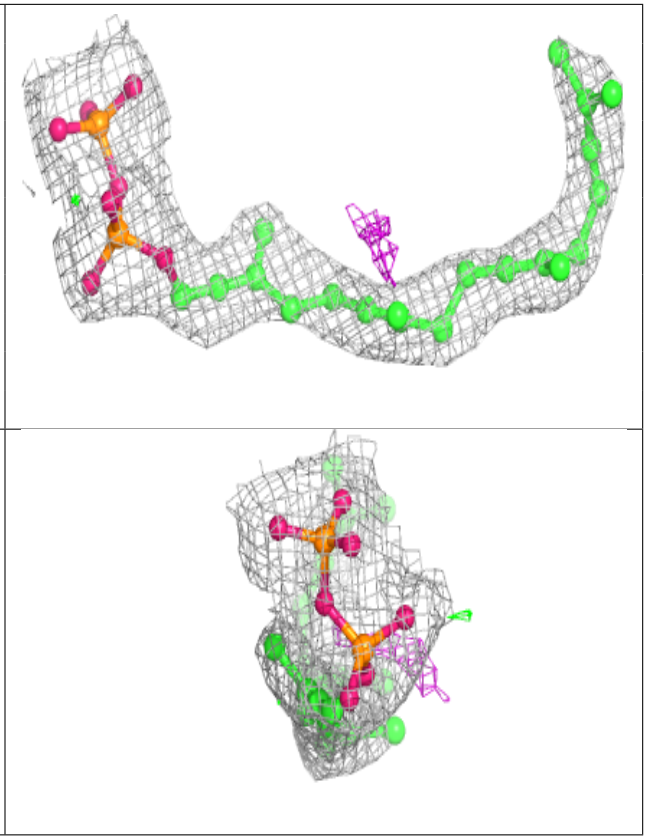
Electron density around GRG A 1502:

$2mF_o$-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.