



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:05 PM UTC

PDB ID : 3CC9 / pdb_00003cc9
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.; 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 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

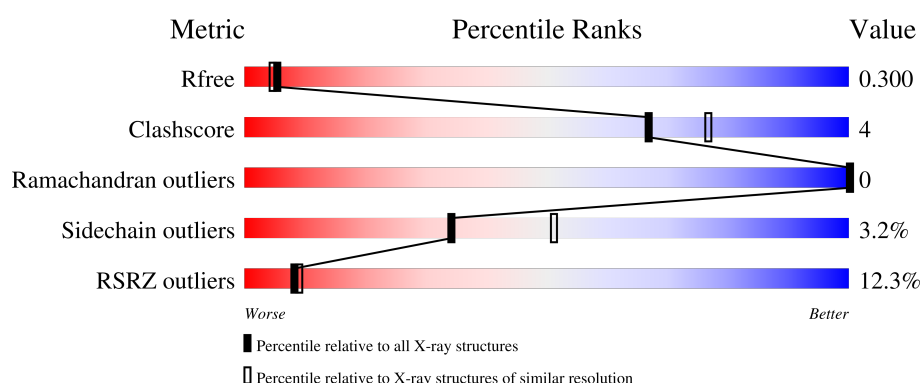
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	396	12% 73% 13% • 13%
1	B	396	8% 83% 7% 10%
1	C	396	13% 76% 8% 16%
1	D	396	11% 78% 6% • 15%

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

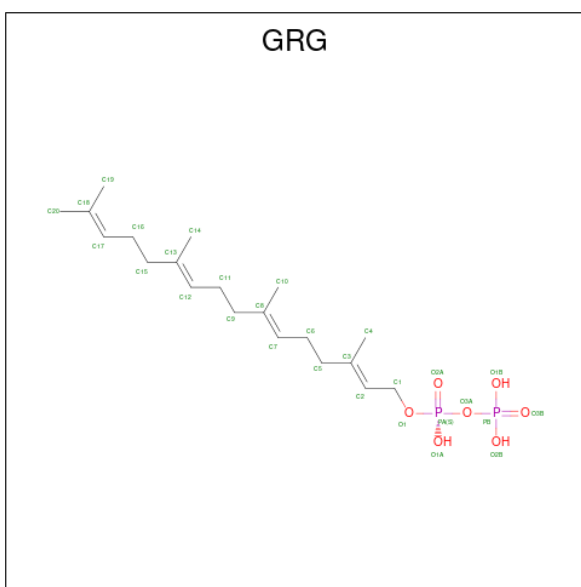
Continued from previous page...

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 (CCD ID: NA) (formula: Na).

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

- Molecule 3 is GERANYLGERANYL DIPHOSPHATE (CCD ID: 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

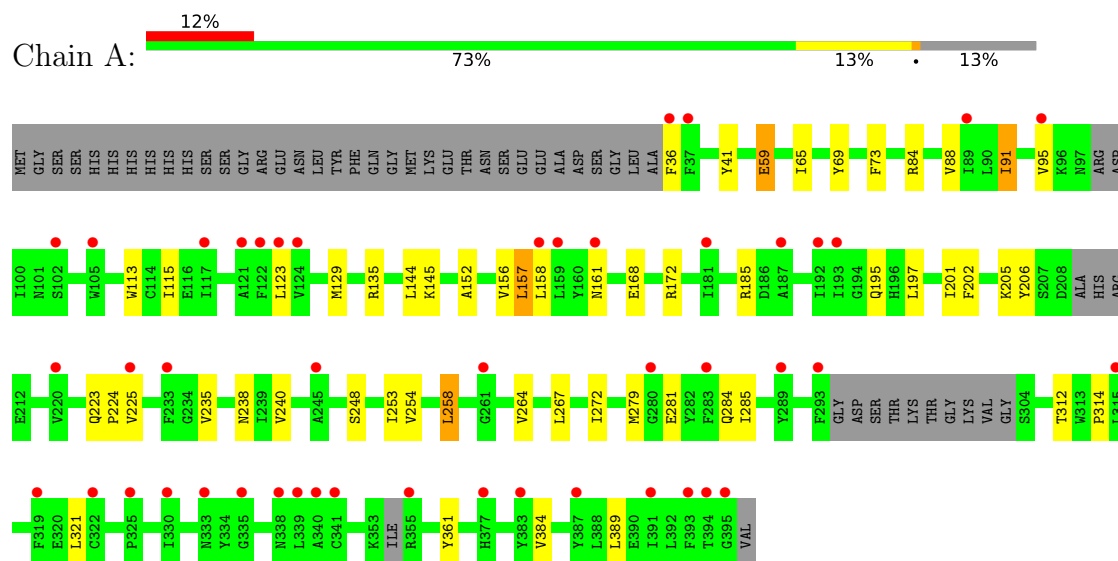
- Molecule 4 is water.

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

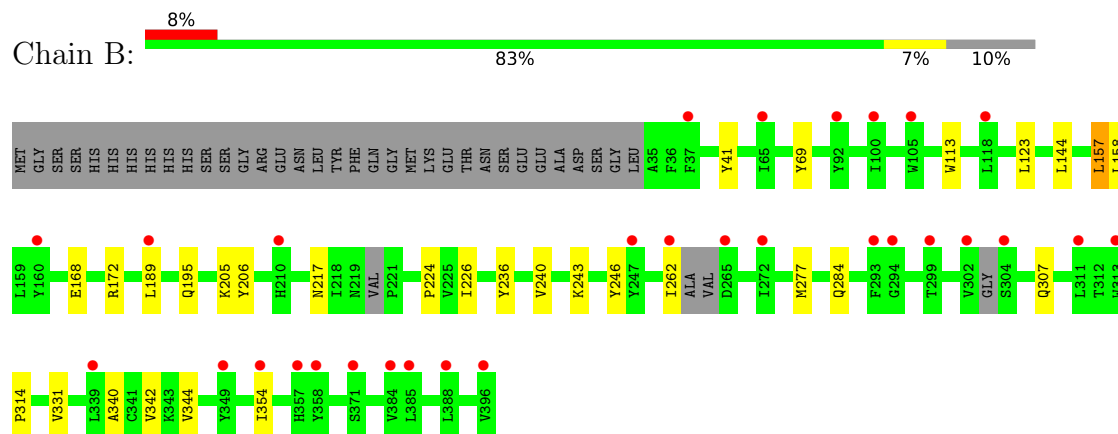
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

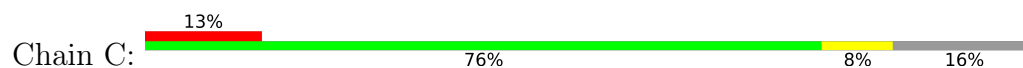
- Molecule 1: Putative farnesyl pyrophosphate synthase

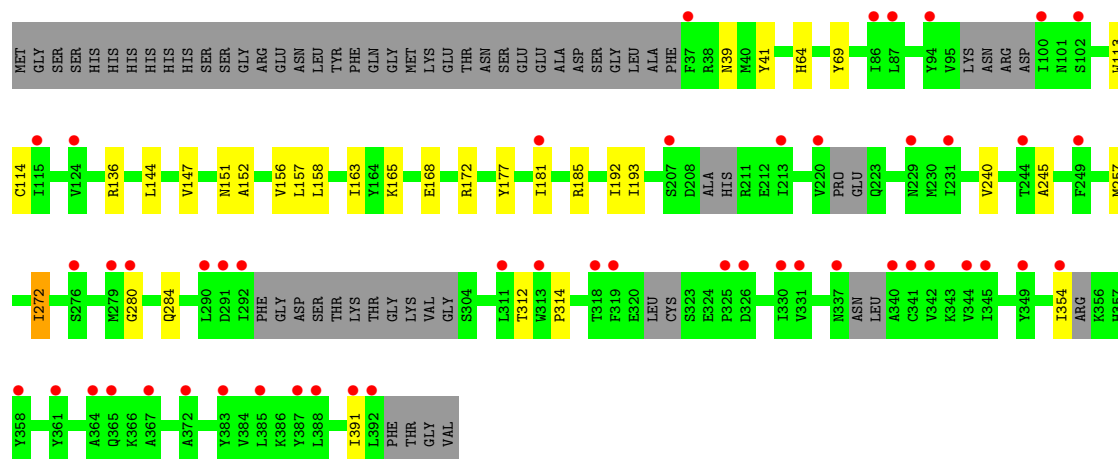


- Molecule 1: Putative farnesyl pyrophosphate synthase

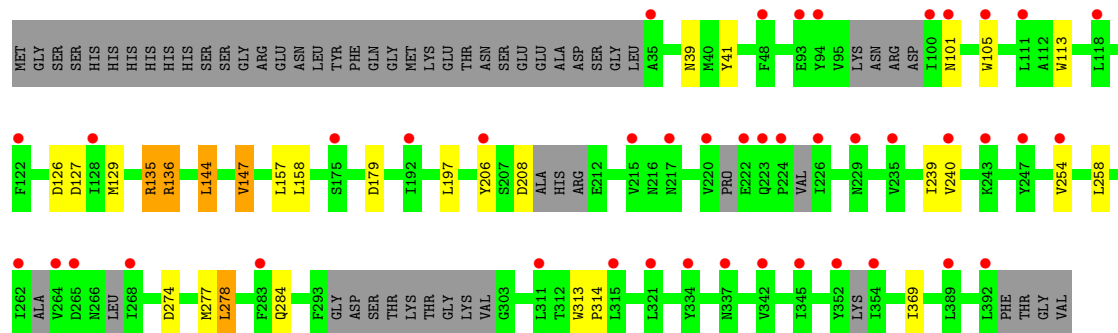
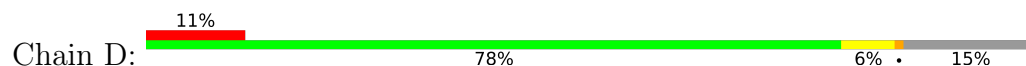


- Molecule 1: Putative farnesyl pyrophosphate synthase





- 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 34.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.61-2.30) 99.6 (34.61-2.30)	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 (Not available) , 0.300	Depositor DCC
R_{free} test set	3720 reflections (5.02%)	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 , 27.6	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	0.46	0/2821	0.84	0/3829
1	B	0.47	0/2952	0.84	0/3999
1	C	0.43	0/2626	0.83	0/3569
1	D	0.44	0/2687	0.85	1/3644 (0.0%)
All	All	0.45	0/11086	0.84	1/15041 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	101	ASN	N-CA-C	5.68	118.82	110.59

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	32	0
1	B	2885	0	2749	19	0
1	C	2578	0	2319	17	0
1	D	2639	0	2417	15	0
2	A	1	0	0	0	0
3	A	29	0	21	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	78	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 (78) 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:59[A]:GLU:H	1:A:59[A]:GLU:CD	1.98	0.71
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:129:MET:HE3	1:A:195:GLN:HE21	1.78	0.47
1:D:126:ASP:HA	1:D:129:MET:HE3	1.96	0.47
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: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:B:246:TYR:OH	1:B:277:MET:HE1	2.18	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:D:274:ASP:HA	1:D:277:MET:HE3	1.99	0.43
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:279:MET:HE3	1:A:389:LEU:HD13	2.03	0.41
1:A:69:TYR:O	1:A:73:PHE:HD2	2.03	0.41
1:C:391:ILE:HG22	1:C:391:ILE:O	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
1:A:59[A]:GLU:CD	1:A:59[A]:GLU:N	2.75	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	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 [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	277/357 (78%)	264 (95%)	13 (5%)	23	35
1	B	294/357 (82%)	288 (98%)	6 (2%)	48	67
1	C	235/357 (66%)	228 (97%)	7 (3%)	36	53
1	D	255/357 (71%)	246 (96%)	9 (4%)	32	48
All	All	1061/1428 (74%)	1026 (97%)	35 (3%)	34	50

All (35) 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	91	ILE
1	A	144	LEU
1	A	157	LEU
1	A	185	ARG
1	A	258	LEU
1	A	264	VAL
1	A	267	LEU
1	A	272	ILE
1	A	321	LEU
1	B	123	LEU
1	B	144	LEU
1	B	157	LEU
1	B	262	ILE
1	B	307	GLN
1	B	342	VAL
1	C	39	ASN
1	C	144	LEU
1	C	157	LEU
1	C	165	LYS
1	C	185	ARG
1	C	193	ILE
1	C	272	ILE
1	D	39	ASN
1	D	105	TRP
1	D	135	ARG
1	D	136	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	144	LEU
1	D	147	VAL
1	D	157	LEU
1	D	208	ASP
1	D	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	333	ASN
1	B	82	ASN
1	B	161	ASN
1	B	195	GLN
1	C	64	HIS
1	C	82	ASN
1	C	173	ASN
1	C	266	ASN
1	D	64	HIS
1	D	195	GLN
1	D	238	ASN
1	D	266	ASN

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](#)

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	B	501	-	27,28,28	3.15	7 (25%)	33,37,37	7.18	10 (30%)
3	GRG	A	501	-	27,28,28	3.23	8 (29%)	33,37,37	7.67	10 (30%)
3	GRG	C	501	-	25,26,28	3.27	8 (32%)	30,34,37	8.31	8 (26%)
3	GRG	D	501	-	27,28,28	3.14	8 (29%)	33,37,37	6.80	8 (24%)

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

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	GRG	C1-C2	-8.28	1.25	1.49
3	A	501	GRG	C1-C2	-8.14	1.26	1.49
3	C	501	GRG	C11-C12	-8.09	1.26	1.50
3	C	501	GRG	C6-C7	-8.05	1.26	1.50
3	D	501	GRG	C11-C12	-8.03	1.26	1.50
3	A	501	GRG	C11-C12	-8.00	1.26	1.50
3	B	501	GRG	C6-C7	-7.93	1.26	1.50
3	A	501	GRG	C6-C7	-7.75	1.27	1.50
3	D	501	GRG	C1-C2	-7.71	1.27	1.49
3	B	501	GRG	C1-C2	-7.62	1.27	1.49
3	B	501	GRG	C11-C12	-7.55	1.27	1.50
3	D	501	GRG	C6-C7	-7.36	1.28	1.50
3	B	501	GRG	C16-C17	-7.33	1.28	1.50
3	D	501	GRG	C16-C17	-6.83	1.29	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GRG	C16-C17	-6.79	1.29	1.50
3	C	501	GRG	C16-C17	-5.15	1.26	1.49
3	A	501	GRG	PA-O3A	3.42	1.63	1.59
3	C	501	GRG	C2-C3	-3.12	1.25	1.33
3	C	501	GRG	C7-C8	-3.09	1.26	1.33
3	D	501	GRG	C12-C13	-3.09	1.26	1.33
3	C	501	GRG	C12-C13	-3.05	1.26	1.33
3	D	501	GRG	C2-C3	-3.04	1.26	1.33
3	A	501	GRG	C7-C8	-3.01	1.26	1.33
3	A	501	GRG	C12-C13	-3.01	1.26	1.33
3	D	501	GRG	C7-C8	-2.93	1.26	1.33
3	A	501	GRG	C2-C3	-2.93	1.26	1.33
3	B	501	GRG	C7-C8	-2.87	1.26	1.33
3	B	501	GRG	C2-C3	-2.85	1.26	1.33
3	C	501	GRG	PA-O3A	2.76	1.62	1.59
3	B	501	GRG	C12-C13	-2.67	1.26	1.33
3	D	501	GRG	PA-O3A	2.44	1.62	1.59

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GRG	C1-C2-C3	32.24	179.02	126.20
3	C	501	GRG	C1-C2-C3	31.92	178.49	126.20
3	B	501	GRG	C1-C2-C3	26.58	169.74	126.20
3	D	501	GRG	C1-C2-C3	25.46	167.91	126.20
3	C	501	GRG	C6-C7-C8	22.53	179.21	127.62
3	C	501	GRG	C11-C12-C13	20.93	175.53	127.62
3	D	501	GRG	C11-C12-C13	20.88	175.41	127.62
3	B	501	GRG	C11-C12-C13	20.13	173.70	127.62
3	A	501	GRG	C11-C12-C13	19.81	172.97	127.62
3	B	501	GRG	C6-C7-C8	19.45	172.14	127.62
3	A	501	GRG	C6-C7-C8	18.36	169.65	127.62
3	D	501	GRG	C6-C7-C8	16.56	165.54	127.62
3	B	501	GRG	C16-C17-C18	11.80	166.98	127.64
3	D	501	GRG	C16-C17-C18	10.24	161.79	127.64
3	A	501	GRG	C16-C17-C18	10.18	161.60	127.64
3	C	501	GRG	C16-C17-C18	6.22	172.04	126.65
3	C	501	GRG	C4-C3-C5	4.11	122.36	115.23
3	B	501	GRG	C4-C3-C5	3.92	122.03	115.23
3	D	501	GRG	C4-C3-C5	3.47	121.26	115.23
3	A	501	GRG	C4-C3-C5	3.46	121.23	115.23
3	D	501	GRG	C14-C13-C15	3.46	121.23	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	GRG	C14-C13-C15	3.37	121.08	115.23
3	A	501	GRG	C14-C13-C15	3.33	121.01	115.23
3	B	501	GRG	C10-C8-C9	2.96	120.36	115.23
3	A	501	GRG	C10-C8-C9	2.88	120.23	115.23
3	C	501	GRG	C10-C8-C9	2.78	120.06	115.23
3	D	501	GRG	C10-C8-C9	2.76	120.03	115.23
3	B	501	GRG	C14-C13-C15	2.61	119.75	115.23
3	A	501	GRG	C15-C16-C17	2.53	124.54	112.02
3	B	501	GRG	C15-C16-C17	2.42	123.97	112.02
3	B	501	GRG	C4-C3-C2	-2.34	117.61	123.63
3	B	501	GRG	C10-C8-C7	-2.33	117.63	123.63
3	C	501	GRG	C15-C16-C17	2.30	120.67	112.95
3	D	501	GRG	C15-C16-C17	2.18	122.79	112.02
3	A	501	GRG	C10-C8-C7	-2.12	118.19	123.63
3	A	501	GRG	C14-C13-C12	-2.10	118.23	123.63

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GRG	C11-C12-C13-C15
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	C1-C2-C3-C5
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-O1-PA-O3A
3	C	501	GRG	C1-O1-PA-O2A
3	D	501	GRG	C11-C12-C13-C14
3	D	501	GRG	C11-C12-C13-C15
3	B	501	GRG	C16-C17-C18-C20
3	A	501	GRG	C4-C3-C5-C6
3	B	501	GRG	C4-C3-C5-C6
3	A	501	GRG	C2-C3-C5-C6
3	B	501	GRG	C2-C3-C5-C6
3	A	501	GRG	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	501	GRG	C6-C7-C8-C10
3	B	501	GRG	C11-C12-C13-C14
3	D	501	GRG	C6-C7-C8-C10
3	A	501	GRG	C6-C7-C8-C9
3	B	501	GRG	C11-C12-C13-C15
3	D	501	GRG	C6-C7-C8-C9
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	B	501	GRG	C12-C11-C9-C8
3	C	501	GRG	C12-C11-C9-C8
3	D	501	GRG	C12-C11-C9-C8
3	B	501	GRG	C13-C15-C16-C17
3	D	501	GRG	C2-C3-C5-C6
3	D	501	GRG	C4-C3-C5-C6
3	C	501	GRG	C1-C2-C3-C4
3	C	501	GRG	C1-C2-C3-C5
3	D	501	GRG	PA-O3A-PB-O2B
3	C	501	GRG	C1-O1-PA-O1A
3	B	501	GRG	C1-C2-C3-C4
3	C	501	GRG	C15-C16-C17-C18
3	A	501	GRG	PB-O3A-PA-O1A
3	D	501	GRG	C5-C6-C7-C8
3	D	501	GRG	C1-C2-C3-C4

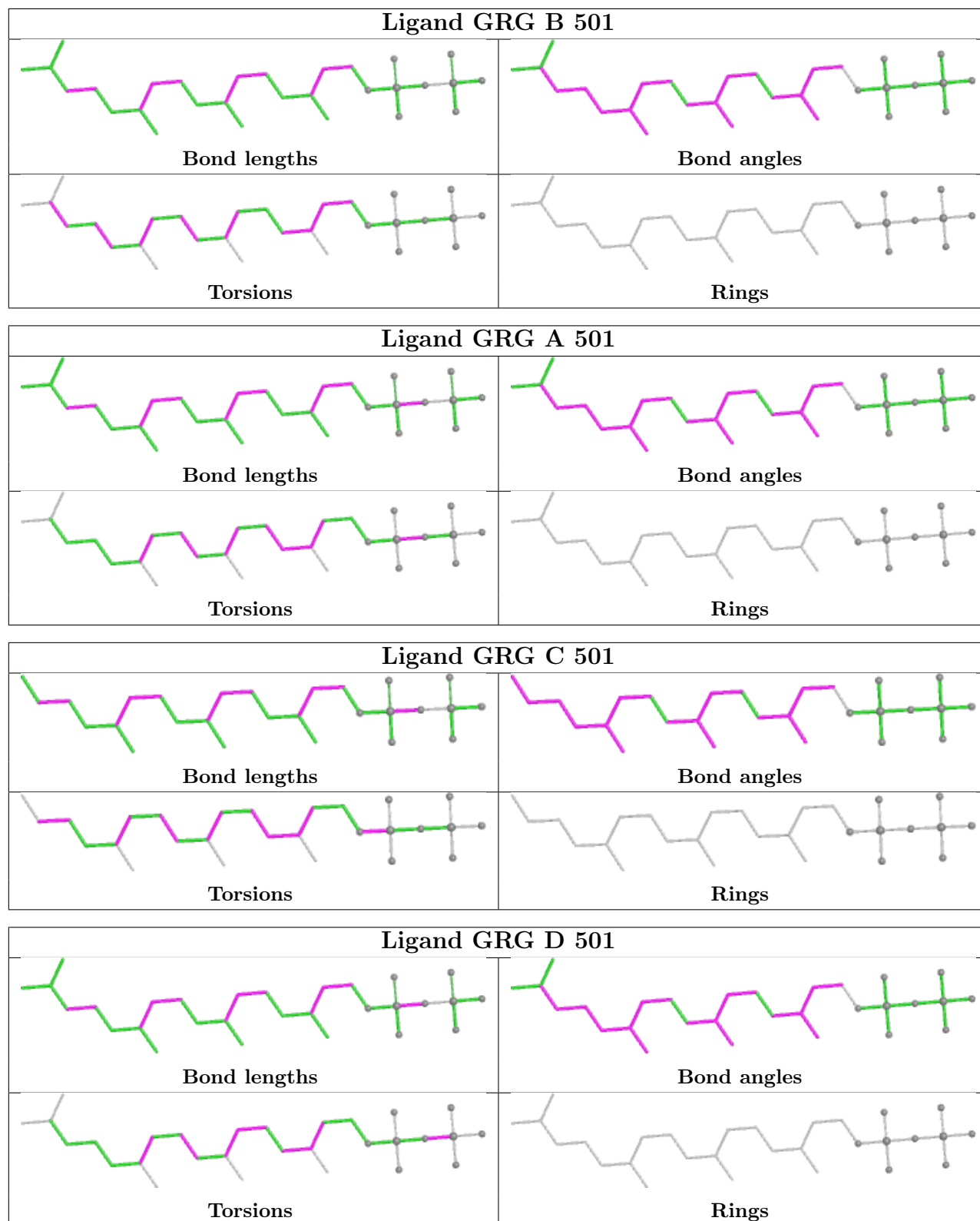
There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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%)	1.05	46 (13%) 7 8	29, 57, 70, 76	2 (0%)
1	B	358/396 (90%)	1.03	30 (8%) 17 18	33, 57, 70, 80	2 (0%)
1	C	332/396 (83%)	1.18	50 (15%) 5 6	49, 65, 77, 91	0
1	D	337/396 (85%)	1.13	43 (12%) 7 8	50, 61, 77, 110	0
All	All	1371/1584 (86%)	1.10	169 (12%) 8 9	29, 59, 75, 110	4 (0%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	302	VAL	6.2
1	D	206	TYR	4.2
1	A	319	PHE	4.1
1	B	37	PHE	4.1
1	C	342	VAL	4.1
1	A	394	THR	4.0
1	C	387	TYR	3.9
1	D	224	PRO	3.8
1	C	292	ILE	3.8
1	D	392	LEU	3.8
1	C	94	TYR	3.8
1	C	290	LEU	3.7
1	C	37	PHE	3.6
1	A	338	ASN	3.6
1	C	383	TYR	3.6
1	A	280	GLY	3.6
1	D	268	ILE	3.5
1	A	395	GLY	3.5
1	D	215	VAL	3.4
1	B	304	SER	3.4
1	B	349	TYR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	35	ALA	3.4
1	B	262	ILE	3.3
1	A	36	PHE	3.3
1	C	325	PRO	3.3
1	D	111	LEU	3.2
1	D	222	GLU	3.2
1	D	334	TYR	3.1
1	C	291	ASP	3.1
1	C	220	VAL	3.1
1	D	352	TYR	3.0
1	A	393	PHE	3.0
1	B	293	PHE	3.0
1	D	101	ASN	3.0
1	C	349	TYR	3.0
1	B	354	ILE	3.0
1	A	89	ILE	3.0
1	B	265	ASP	3.0
1	D	105	TRP	2.9
1	A	391	ILE	2.9
1	C	311	LEU	2.9
1	B	313	TRP	2.9
1	A	158	LEU	2.8
1	B	311	LEU	2.8
1	B	396	VAL	2.8
1	A	105	TRP	2.8
1	C	313	TRP	2.8
1	A	333	ASN	2.8
1	D	235	VAL	2.8
1	D	254	VAL	2.8
1	C	345	ILE	2.8
1	C	388	LEU	2.8
1	C	364	ALA	2.8
1	D	264	VAL	2.8
1	C	244	THR	2.8
1	D	345	ILE	2.7
1	A	117	ILE	2.7
1	C	319	PHE	2.7
1	B	299	THR	2.7
1	A	325	PRO	2.7
1	A	340	ALA	2.6
1	B	92	TYR	2.6
1	C	318	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	65	ILE	2.6
1	C	391	ILE	2.6
1	D	100	ILE	2.6
1	A	341	CYS	2.6
1	A	220	VAL	2.6
1	A	322	CYS	2.6
1	C	337	ASN	2.6
1	A	124	VAL	2.6
1	C	280	GLY	2.6
1	C	361	TYR	2.6
1	D	220	VAL	2.6
1	D	226	ILE	2.6
1	C	115	ILE	2.6
1	A	315	LEU	2.5
1	B	294	GLY	2.5
1	C	207	SER	2.5
1	C	358	TYR	2.5
1	B	388	LEU	2.5
1	D	315	LEU	2.5
1	A	121	ALA	2.5
1	A	123	LEU	2.5
1	D	311	LEU	2.5
1	A	339	LEU	2.4
1	D	247	TYR	2.4
1	D	175	SER	2.4
1	A	293	PHE	2.4
1	C	86	ILE	2.4
1	D	240	VAL	2.4
1	D	342	VAL	2.4
1	D	354	ILE	2.4
1	B	210[A]	HIS	2.4
1	D	262	ILE	2.4
1	A	387	TYR	2.3
1	A	335	GLY	2.3
1	A	192	ILE	2.3
1	D	118	LEU	2.3
1	D	337	ASN	2.3
1	A	261	GLY	2.3
1	B	357	HIS	2.3
1	C	354	ILE	2.3
1	A	122	PHE	2.3
1	C	249	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	341	CYS	2.3
1	B	105	TRP	2.3
1	C	340	ALA	2.3
1	B	371	SER	2.3
1	C	102	SER	2.3
1	A	283	PHE	2.3
1	C	124	VAL	2.3
1	D	243	LYS	2.3
1	C	229	ASN	2.3
1	C	276	SER	2.3
1	D	223	GLN	2.3
1	A	181	ILE	2.3
1	C	87	LEU	2.2
1	C	392	LEU	2.2
1	A	355	ARG	2.2
1	C	367	ALA	2.2
1	C	365	GLN	2.2
1	D	128	ILE	2.2
1	C	385	LEU	2.2
1	A	233	PHE	2.2
1	D	229	ASN	2.2
1	B	272	ILE	2.2
1	C	330	ILE	2.2
1	B	384	VAL	2.2
1	D	122	PHE	2.2
1	D	321	LEU	2.2
1	A	95	VAL	2.2
1	D	93	GLU	2.2
1	A	245	ALA	2.2
1	C	372	ALA	2.2
1	B	358	TYR	2.1
1	A	159	LEU	2.1
1	B	100	ILE	2.1
1	B	189	LEU	2.1
1	B	339	LEU	2.1
1	C	181	ILE	2.1
1	C	326	ASP	2.1
1	D	48	PHE	2.1
1	D	283	PHE	2.1
1	A	289	TYR	2.1
1	A	193	ILE	2.1
1	C	231	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	279	MET	2.1
1	A	161	ASN	2.1
1	A	102	SER	2.1
1	B	385	LEU	2.1
1	A	383	TYR	2.1
1	C	213	ILE	2.1
1	D	265	ASP	2.1
1	A	187	ALA	2.1
1	B	118	LEU	2.1
1	B	247	TYR	2.1
1	C	344	VAL	2.1
1	D	217	ASN	2.0
1	A	330	ILE	2.0
1	C	100	ILE	2.0
1	D	192	ILE	2.0
1	B	160	TYR	2.0
1	D	94	TYR	2.0
1	A	225	VAL	2.0
1	C	331	VAL	2.0
1	A	37	PHE	2.0
1	A	377	HIS	2.0
1	D	389	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GRG	C	501	27/29	0.89	0.15	67,70,74,75	0

Continued on next page...

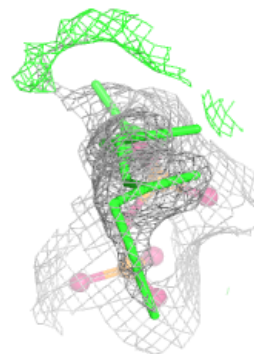
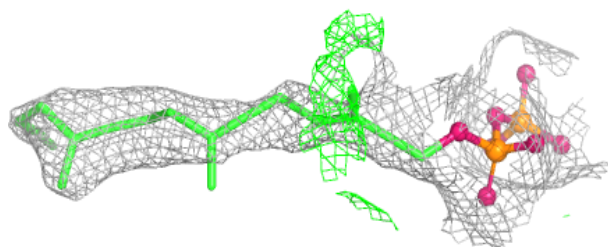
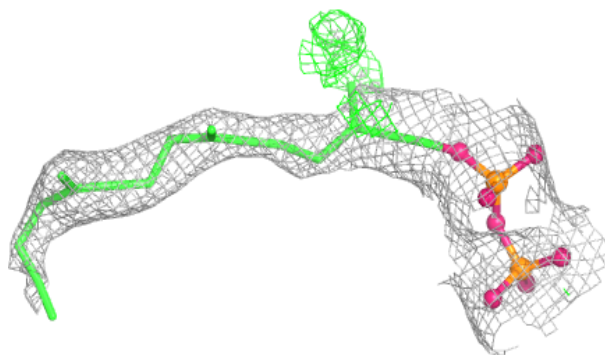
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GRG	D	501	29/29	0.91	0.20	38,49,65,65	20
2	NA	A	502	1/1	0.94	0.07	54,54,54,54	0
3	GRG	A	501	29/29	0.95	0.10	43,48,54,55	0
3	GRG	B	501	29/29	0.95	0.11	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.

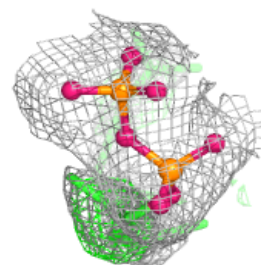
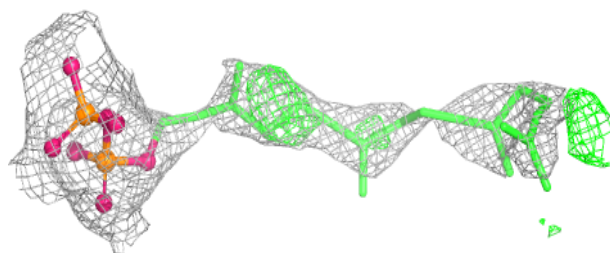
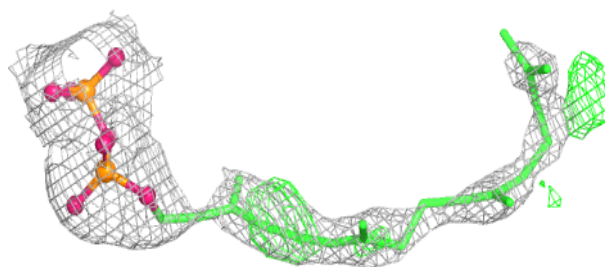
Electron density around GRG C 501:

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

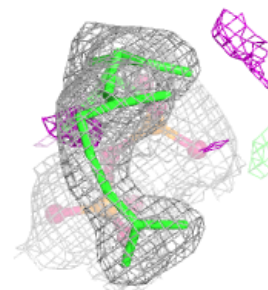
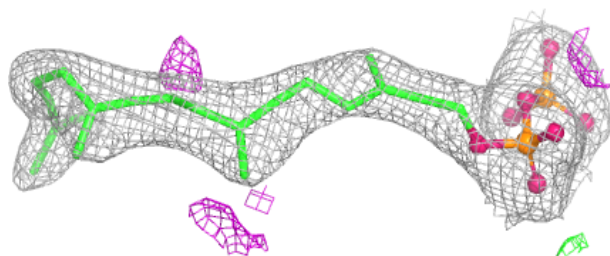
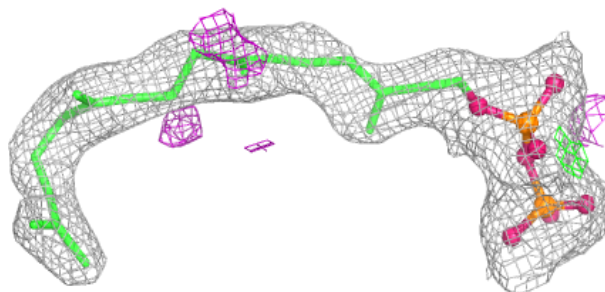


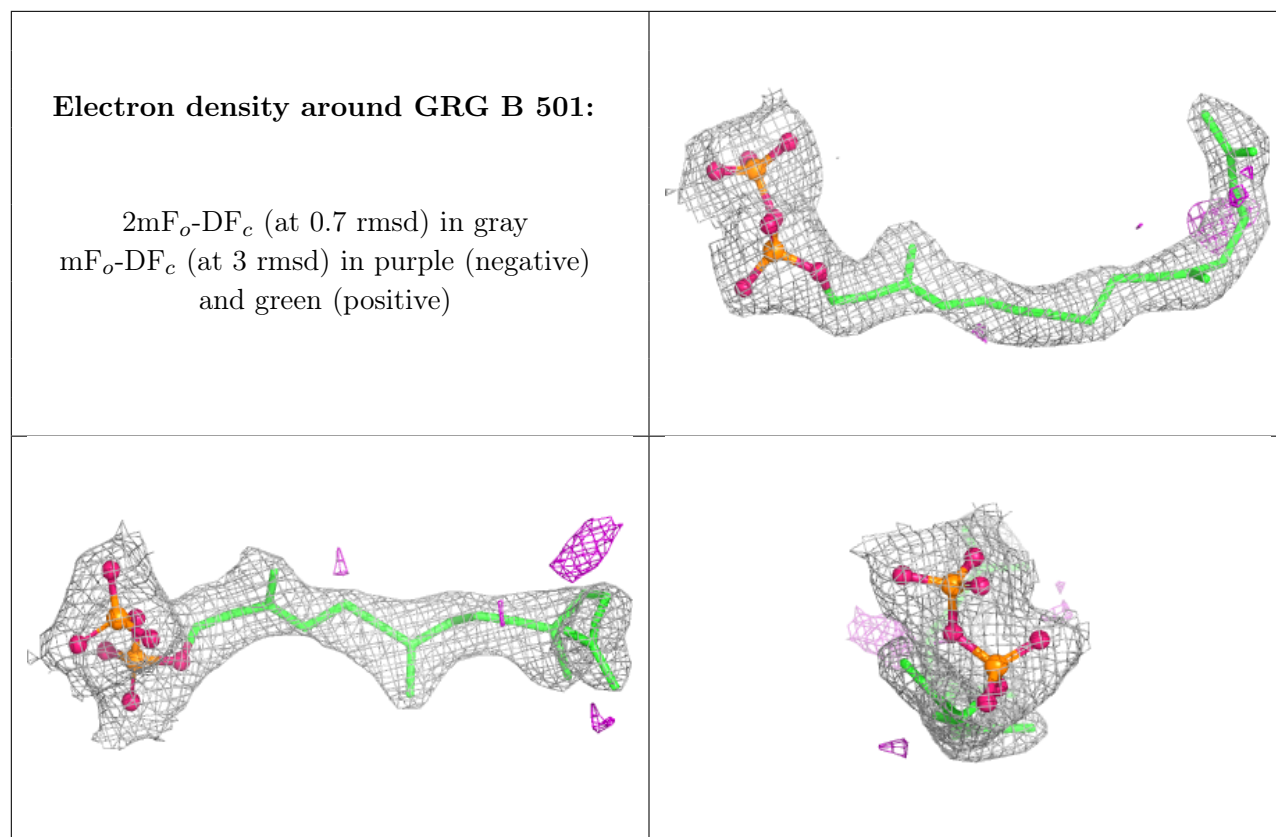
Electron density around GRG D 501:

$2mF_o-DF_c$ (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.