



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 07:45 am GMT

PDB ID : 6R4N
Title : Crystal structure of *S. cerevisia* Niemann-Pick type C protein NPC2 with ergosterol bound
Authors : Winkler, M.B.L.; Kidmose, R.T.; Pedersen, B.P.
Deposited on : 2019-03-22
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

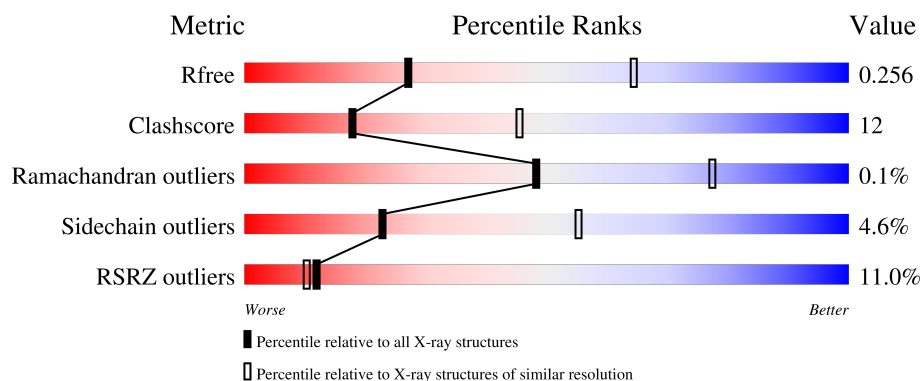
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



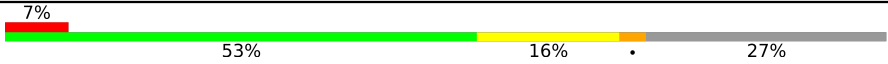

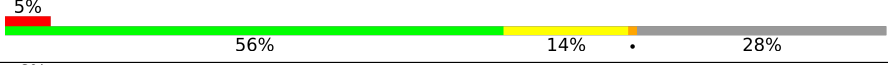

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	201	
1	B	201	
1	C	201	
1	D	201	
1	E	201	

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Mol	Chain	Length	Quality of chain
1	F	201	
1	G	201	
1	H	201	
1	I	201	
2	J	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10486 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 Phosphatidylglycerol/phosphatidylinositol transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1125	717	177	227	4			
1	B	141	Total	C	N	O	S	0	0	0
			1103	701	174	224	4			
1	C	147	Total	C	N	O	S	0	0	0
			1150	733	183	230	4			
1	D	142	Total	C	N	O	S	0	0	0
			1106	705	172	225	4			
1	E	143	Total	C	N	O	S	0	0	0
			1118	712	176	226	4			
1	F	146	Total	C	N	O	S	0	0	0
			1139	727	179	229	4			
1	G	144	Total	C	N	O	S	0	0	0
			1125	717	177	227	4			
1	H	145	Total	C	N	O	S	0	0	0
			1130	720	178	228	4			
1	I	144	Total	C	N	O	S	0	0	0
			1125	717	177	227	4			

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	174	LEU	-	expression tag	UNP Q12408
A	175	VAL	-	expression tag	UNP Q12408
A	176	PRO	-	expression tag	UNP Q12408
A	177	ARG	-	expression tag	UNP Q12408
A	178	GLY	-	expression tag	UNP Q12408
A	179	SER	-	expression tag	UNP Q12408
A	180	GLY	-	expression tag	UNP Q12408
A	181	GLY	-	expression tag	UNP Q12408
A	182	GLY	-	expression tag	UNP Q12408
A	183	GLY	-	expression tag	UNP Q12408
A	184	SER	-	expression tag	UNP Q12408

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Chain	Residue	Modelled	Actual	Comment	Reference
A	185	GLY	-	expression tag	UNP Q12408
A	186	GLY	-	expression tag	UNP Q12408
A	187	GLY	-	expression tag	UNP Q12408
A	188	GLY	-	expression tag	UNP Q12408
A	189	SER	-	expression tag	UNP Q12408
A	190	GLY	-	expression tag	UNP Q12408
A	191	GLY	-	expression tag	UNP Q12408
A	192	HIS	-	expression tag	UNP Q12408
A	193	HIS	-	expression tag	UNP Q12408
A	194	HIS	-	expression tag	UNP Q12408
A	195	HIS	-	expression tag	UNP Q12408
A	196	HIS	-	expression tag	UNP Q12408
A	197	HIS	-	expression tag	UNP Q12408
A	198	HIS	-	expression tag	UNP Q12408
A	199	HIS	-	expression tag	UNP Q12408
A	200	HIS	-	expression tag	UNP Q12408
A	201	HIS	-	expression tag	UNP Q12408
B	174	LEU	-	expression tag	UNP Q12408
B	175	VAL	-	expression tag	UNP Q12408
B	176	PRO	-	expression tag	UNP Q12408
B	177	ARG	-	expression tag	UNP Q12408
B	178	GLY	-	expression tag	UNP Q12408
B	179	SER	-	expression tag	UNP Q12408
B	180	GLY	-	expression tag	UNP Q12408
B	181	GLY	-	expression tag	UNP Q12408
B	182	GLY	-	expression tag	UNP Q12408
B	183	GLY	-	expression tag	UNP Q12408
B	184	SER	-	expression tag	UNP Q12408
B	185	GLY	-	expression tag	UNP Q12408
B	186	GLY	-	expression tag	UNP Q12408
B	187	GLY	-	expression tag	UNP Q12408
B	188	GLY	-	expression tag	UNP Q12408
B	189	SER	-	expression tag	UNP Q12408
B	190	GLY	-	expression tag	UNP Q12408
B	191	GLY	-	expression tag	UNP Q12408
B	192	HIS	-	expression tag	UNP Q12408
B	193	HIS	-	expression tag	UNP Q12408
B	194	HIS	-	expression tag	UNP Q12408
B	195	HIS	-	expression tag	UNP Q12408
B	196	HIS	-	expression tag	UNP Q12408
B	197	HIS	-	expression tag	UNP Q12408
B	198	HIS	-	expression tag	UNP Q12408

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Chain	Residue	Modelled	Actual	Comment	Reference
B	199	HIS	-	expression tag	UNP Q12408
B	200	HIS	-	expression tag	UNP Q12408
B	201	HIS	-	expression tag	UNP Q12408
C	174	LEU	-	expression tag	UNP Q12408
C	175	VAL	-	expression tag	UNP Q12408
C	176	PRO	-	expression tag	UNP Q12408
C	177	ARG	-	expression tag	UNP Q12408
C	178	GLY	-	expression tag	UNP Q12408
C	179	SER	-	expression tag	UNP Q12408
C	180	GLY	-	expression tag	UNP Q12408
C	181	GLY	-	expression tag	UNP Q12408
C	182	GLY	-	expression tag	UNP Q12408
C	183	GLY	-	expression tag	UNP Q12408
C	184	SER	-	expression tag	UNP Q12408
C	185	GLY	-	expression tag	UNP Q12408
C	186	GLY	-	expression tag	UNP Q12408
C	187	GLY	-	expression tag	UNP Q12408
C	188	GLY	-	expression tag	UNP Q12408
C	189	SER	-	expression tag	UNP Q12408
C	190	GLY	-	expression tag	UNP Q12408
C	191	GLY	-	expression tag	UNP Q12408
C	192	HIS	-	expression tag	UNP Q12408
C	193	HIS	-	expression tag	UNP Q12408
C	194	HIS	-	expression tag	UNP Q12408
C	195	HIS	-	expression tag	UNP Q12408
C	196	HIS	-	expression tag	UNP Q12408
C	197	HIS	-	expression tag	UNP Q12408
C	198	HIS	-	expression tag	UNP Q12408
C	199	HIS	-	expression tag	UNP Q12408
C	200	HIS	-	expression tag	UNP Q12408
C	201	HIS	-	expression tag	UNP Q12408
D	174	LEU	-	expression tag	UNP Q12408
D	175	VAL	-	expression tag	UNP Q12408
D	176	PRO	-	expression tag	UNP Q12408
D	177	ARG	-	expression tag	UNP Q12408
D	178	GLY	-	expression tag	UNP Q12408
D	179	SER	-	expression tag	UNP Q12408
D	180	GLY	-	expression tag	UNP Q12408
D	181	GLY	-	expression tag	UNP Q12408
D	182	GLY	-	expression tag	UNP Q12408
D	183	GLY	-	expression tag	UNP Q12408
D	184	SER	-	expression tag	UNP Q12408

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Chain	Residue	Modelled	Actual	Comment	Reference
D	185	GLY	-	expression tag	UNP Q12408
D	186	GLY	-	expression tag	UNP Q12408
D	187	GLY	-	expression tag	UNP Q12408
D	188	GLY	-	expression tag	UNP Q12408
D	189	SER	-	expression tag	UNP Q12408
D	190	GLY	-	expression tag	UNP Q12408
D	191	GLY	-	expression tag	UNP Q12408
D	192	HIS	-	expression tag	UNP Q12408
D	193	HIS	-	expression tag	UNP Q12408
D	194	HIS	-	expression tag	UNP Q12408
D	195	HIS	-	expression tag	UNP Q12408
D	196	HIS	-	expression tag	UNP Q12408
D	197	HIS	-	expression tag	UNP Q12408
D	198	HIS	-	expression tag	UNP Q12408
D	199	HIS	-	expression tag	UNP Q12408
D	200	HIS	-	expression tag	UNP Q12408
D	201	HIS	-	expression tag	UNP Q12408
E	174	LEU	-	expression tag	UNP Q12408
E	175	VAL	-	expression tag	UNP Q12408
E	176	PRO	-	expression tag	UNP Q12408
E	177	ARG	-	expression tag	UNP Q12408
E	178	GLY	-	expression tag	UNP Q12408
E	179	SER	-	expression tag	UNP Q12408
E	180	GLY	-	expression tag	UNP Q12408
E	181	GLY	-	expression tag	UNP Q12408
E	182	GLY	-	expression tag	UNP Q12408
E	183	GLY	-	expression tag	UNP Q12408
E	184	SER	-	expression tag	UNP Q12408
E	185	GLY	-	expression tag	UNP Q12408
E	186	GLY	-	expression tag	UNP Q12408
E	187	GLY	-	expression tag	UNP Q12408
E	188	GLY	-	expression tag	UNP Q12408
E	189	SER	-	expression tag	UNP Q12408
E	190	GLY	-	expression tag	UNP Q12408
E	191	GLY	-	expression tag	UNP Q12408
E	192	HIS	-	expression tag	UNP Q12408
E	193	HIS	-	expression tag	UNP Q12408
E	194	HIS	-	expression tag	UNP Q12408
E	195	HIS	-	expression tag	UNP Q12408
E	196	HIS	-	expression tag	UNP Q12408
E	197	HIS	-	expression tag	UNP Q12408
E	198	HIS	-	expression tag	UNP Q12408

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Chain	Residue	Modelled	Actual	Comment	Reference
E	199	HIS	-	expression tag	UNP Q12408
E	200	HIS	-	expression tag	UNP Q12408
E	201	HIS	-	expression tag	UNP Q12408
F	174	LEU	-	expression tag	UNP Q12408
F	175	VAL	-	expression tag	UNP Q12408
F	176	PRO	-	expression tag	UNP Q12408
F	177	ARG	-	expression tag	UNP Q12408
F	178	GLY	-	expression tag	UNP Q12408
F	179	SER	-	expression tag	UNP Q12408
F	180	GLY	-	expression tag	UNP Q12408
F	181	GLY	-	expression tag	UNP Q12408
F	182	GLY	-	expression tag	UNP Q12408
F	183	GLY	-	expression tag	UNP Q12408
F	184	SER	-	expression tag	UNP Q12408
F	185	GLY	-	expression tag	UNP Q12408
F	186	GLY	-	expression tag	UNP Q12408
F	187	GLY	-	expression tag	UNP Q12408
F	188	GLY	-	expression tag	UNP Q12408
F	189	SER	-	expression tag	UNP Q12408
F	190	GLY	-	expression tag	UNP Q12408
F	191	GLY	-	expression tag	UNP Q12408
F	192	HIS	-	expression tag	UNP Q12408
F	193	HIS	-	expression tag	UNP Q12408
F	194	HIS	-	expression tag	UNP Q12408
F	195	HIS	-	expression tag	UNP Q12408
F	196	HIS	-	expression tag	UNP Q12408
F	197	HIS	-	expression tag	UNP Q12408
F	198	HIS	-	expression tag	UNP Q12408
F	199	HIS	-	expression tag	UNP Q12408
F	200	HIS	-	expression tag	UNP Q12408
F	201	HIS	-	expression tag	UNP Q12408
G	174	LEU	-	expression tag	UNP Q12408
G	175	VAL	-	expression tag	UNP Q12408
G	176	PRO	-	expression tag	UNP Q12408
G	177	ARG	-	expression tag	UNP Q12408
G	178	GLY	-	expression tag	UNP Q12408
G	179	SER	-	expression tag	UNP Q12408
G	180	GLY	-	expression tag	UNP Q12408
G	181	GLY	-	expression tag	UNP Q12408
G	182	GLY	-	expression tag	UNP Q12408
G	183	GLY	-	expression tag	UNP Q12408
G	184	SER	-	expression tag	UNP Q12408

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Chain	Residue	Modelled	Actual	Comment	Reference
G	185	GLY	-	expression tag	UNP Q12408
G	186	GLY	-	expression tag	UNP Q12408
G	187	GLY	-	expression tag	UNP Q12408
G	188	GLY	-	expression tag	UNP Q12408
G	189	SER	-	expression tag	UNP Q12408
G	190	GLY	-	expression tag	UNP Q12408
G	191	GLY	-	expression tag	UNP Q12408
G	192	HIS	-	expression tag	UNP Q12408
G	193	HIS	-	expression tag	UNP Q12408
G	194	HIS	-	expression tag	UNP Q12408
G	195	HIS	-	expression tag	UNP Q12408
G	196	HIS	-	expression tag	UNP Q12408
G	197	HIS	-	expression tag	UNP Q12408
G	198	HIS	-	expression tag	UNP Q12408
G	199	HIS	-	expression tag	UNP Q12408
G	200	HIS	-	expression tag	UNP Q12408
G	201	HIS	-	expression tag	UNP Q12408
H	174	LEU	-	expression tag	UNP Q12408
H	175	VAL	-	expression tag	UNP Q12408
H	176	PRO	-	expression tag	UNP Q12408
H	177	ARG	-	expression tag	UNP Q12408
H	178	GLY	-	expression tag	UNP Q12408
H	179	SER	-	expression tag	UNP Q12408
H	180	GLY	-	expression tag	UNP Q12408
H	181	GLY	-	expression tag	UNP Q12408
H	182	GLY	-	expression tag	UNP Q12408
H	183	GLY	-	expression tag	UNP Q12408
H	184	SER	-	expression tag	UNP Q12408
H	185	GLY	-	expression tag	UNP Q12408
H	186	GLY	-	expression tag	UNP Q12408
H	187	GLY	-	expression tag	UNP Q12408
H	188	GLY	-	expression tag	UNP Q12408
H	189	SER	-	expression tag	UNP Q12408
H	190	GLY	-	expression tag	UNP Q12408
H	191	GLY	-	expression tag	UNP Q12408
H	192	HIS	-	expression tag	UNP Q12408
H	193	HIS	-	expression tag	UNP Q12408
H	194	HIS	-	expression tag	UNP Q12408
H	195	HIS	-	expression tag	UNP Q12408
H	196	HIS	-	expression tag	UNP Q12408
H	197	HIS	-	expression tag	UNP Q12408
H	198	HIS	-	expression tag	UNP Q12408

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Chain	Residue	Modelled	Actual	Comment	Reference
H	199	HIS	-	expression tag	UNP Q12408
H	200	HIS	-	expression tag	UNP Q12408
H	201	HIS	-	expression tag	UNP Q12408
I	174	LEU	-	expression tag	UNP Q12408
I	175	VAL	-	expression tag	UNP Q12408
I	176	PRO	-	expression tag	UNP Q12408
I	177	ARG	-	expression tag	UNP Q12408
I	178	GLY	-	expression tag	UNP Q12408
I	179	SER	-	expression tag	UNP Q12408
I	180	GLY	-	expression tag	UNP Q12408
I	181	GLY	-	expression tag	UNP Q12408
I	182	GLY	-	expression tag	UNP Q12408
I	183	GLY	-	expression tag	UNP Q12408
I	184	SER	-	expression tag	UNP Q12408
I	185	GLY	-	expression tag	UNP Q12408
I	186	GLY	-	expression tag	UNP Q12408
I	187	GLY	-	expression tag	UNP Q12408
I	188	GLY	-	expression tag	UNP Q12408
I	189	SER	-	expression tag	UNP Q12408
I	190	GLY	-	expression tag	UNP Q12408
I	191	GLY	-	expression tag	UNP Q12408
I	192	HIS	-	expression tag	UNP Q12408
I	193	HIS	-	expression tag	UNP Q12408
I	194	HIS	-	expression tag	UNP Q12408
I	195	HIS	-	expression tag	UNP Q12408
I	196	HIS	-	expression tag	UNP Q12408
I	197	HIS	-	expression tag	UNP Q12408
I	198	HIS	-	expression tag	UNP Q12408
I	199	HIS	-	expression tag	UNP Q12408
I	200	HIS	-	expression tag	UNP Q12408
I	201	HIS	-	expression tag	UNP Q12408

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



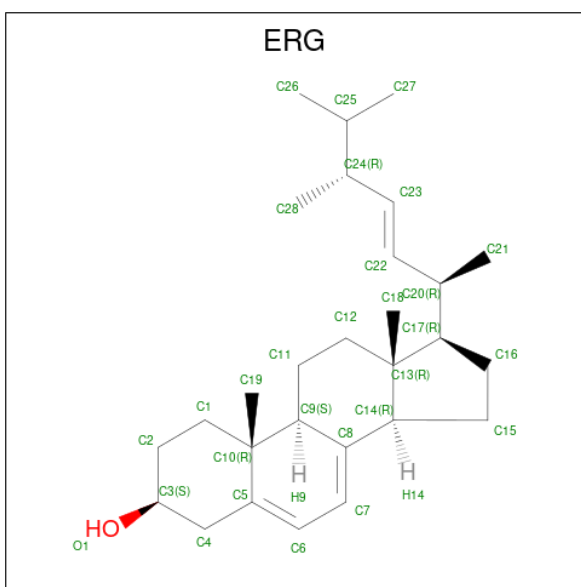
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



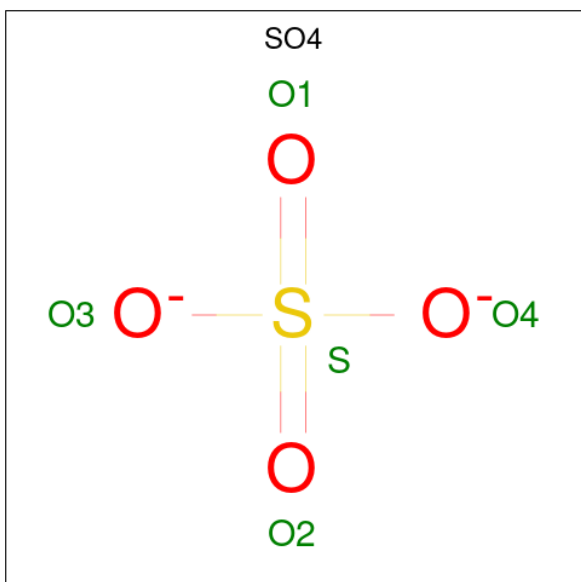
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ERGOSTEROL (three-letter code: ERG) (formula: $C_{28}H_{44}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			29	28	1		
4	C	1	Total	C	O	0	0
			29	28	1		
4	C	1	Total	C	O	0	0
			29	28	1		
4	E	1	Total	C	O	0	0
			29	28	1		
4	I	1	Total	C	O	0	0
			29	28	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

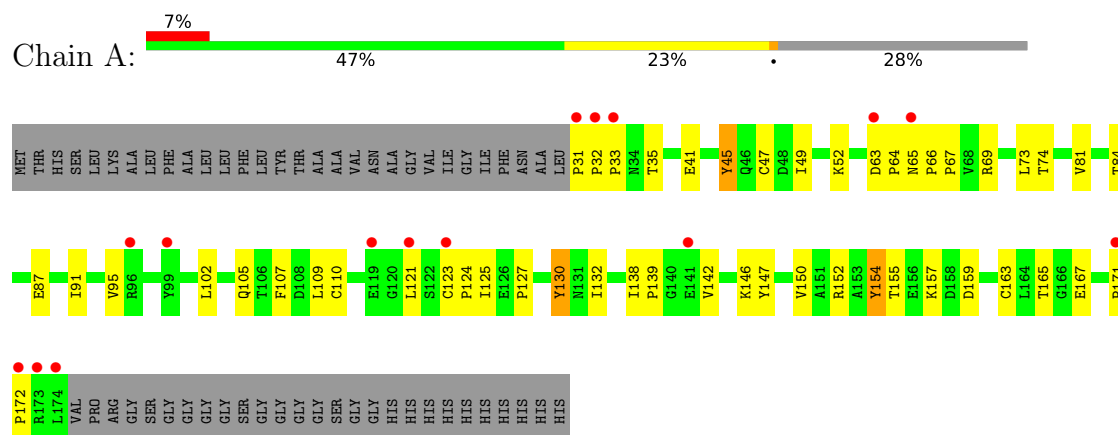


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0

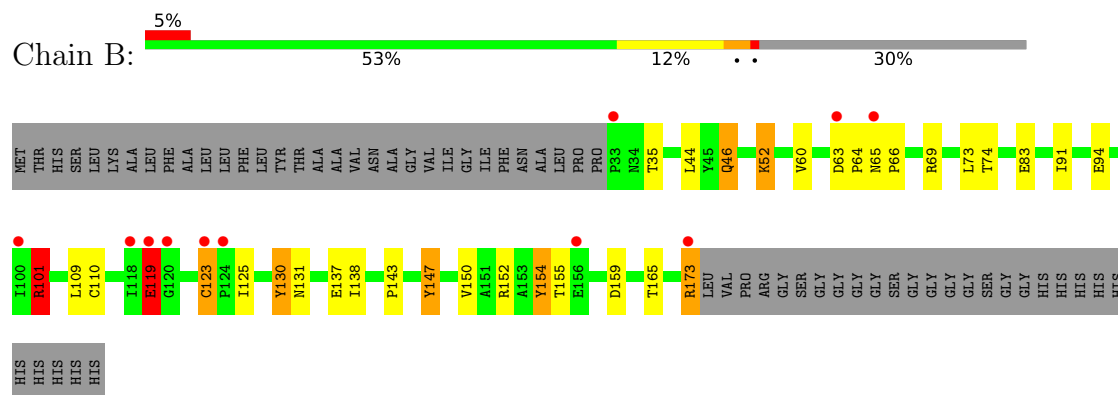
3 Residue-property plots [i](#)

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.

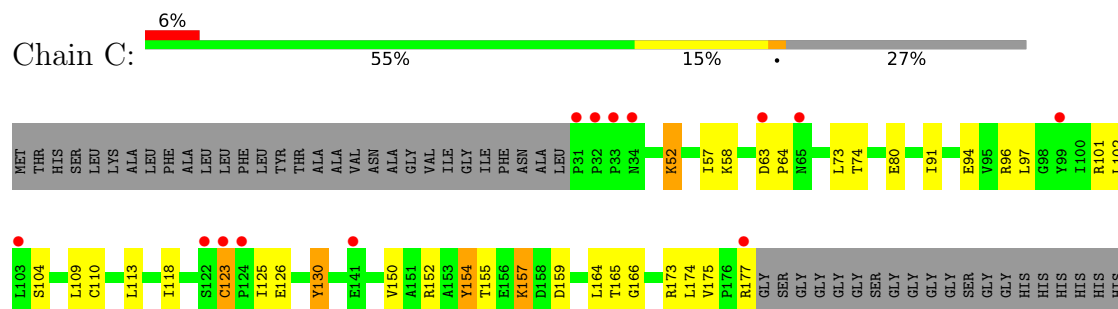
- Molecule 1: Phosphatidylglycerol/phosphatidylinositol transfer protein

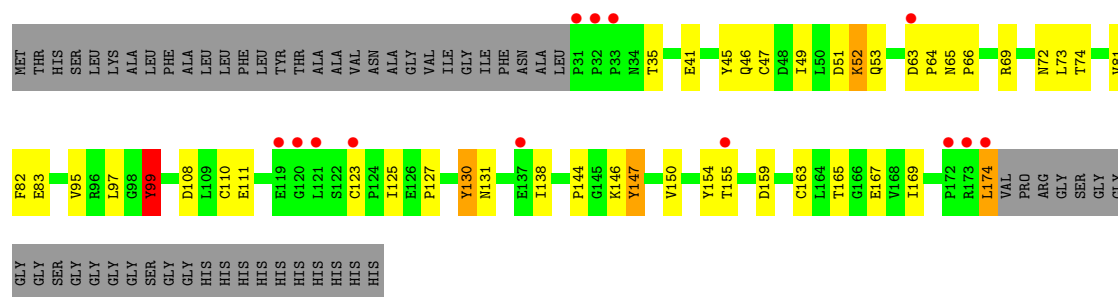


- Molecule 1: Phosphatidylglycerol/phosphatidylinositol transfer protein

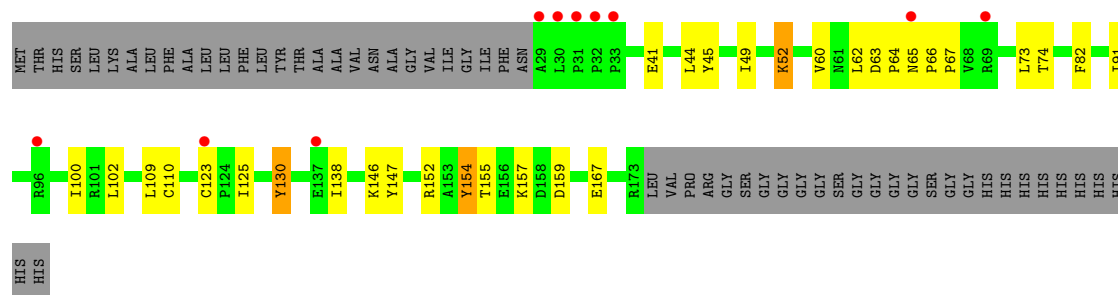


- Molecule 1: Phosphatidylglycerol/phosphatidylinositol transfer protein

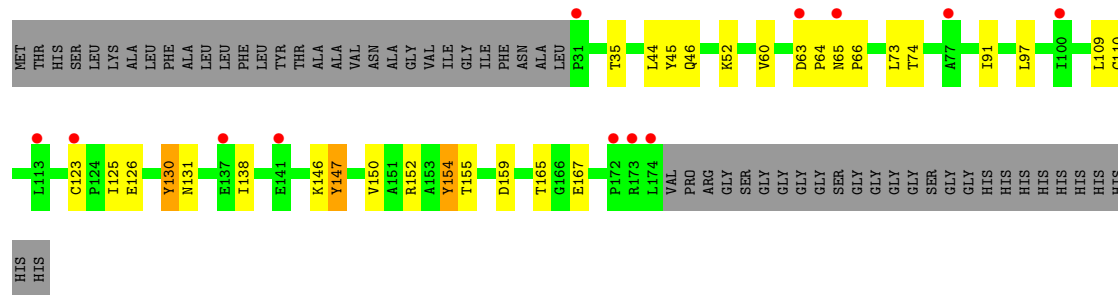




- Molecule 1: Phosphatidylglycerol/phosphatidylinositol transfer protein



- Molecule 1: Phosphatidylglycerol/phosphatidylinositol transfer protein



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	215.39Å 215.39Å 129.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.75 – 2.90 47.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.75-2.90) 100.0 (47.75-2.90)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.257 0.226 , 0.256	Depositor DCC
R_{free} test set	73866 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10486	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: NAG, SO4, ERG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/1148	0.78	0/1568
1	B	0.57	1/1124 (0.1%)	0.88	2/1533 (0.1%)
1	C	0.50	0/1174	0.77	1/1604 (0.1%)
1	D	0.49	0/1129	0.82	4/1543 (0.3%)
1	E	0.50	0/1140	0.83	2/1556 (0.1%)
1	F	0.53	0/1163	0.85	3/1590 (0.2%)
1	G	0.52	0/1148	0.83	1/1568 (0.1%)
1	H	0.49	0/1153	0.79	0/1576
1	I	0.46	0/1148	0.75	0/1568
All	All	0.50	1/10327 (0.0%)	0.81	13/14106 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	119	GLU	CB-CG	6.63	1.64	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	113	LEU	CB-CG-CD2	9.51	127.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	100	ILE	CA-CB-CG1	-8.28	95.27	111.00
1	D	96	ARG	CG-CD-NE	7.90	128.38	111.80
1	D	109	LEU	CB-CG-CD1	6.53	122.11	111.00
1	D	96	ARG	NE-CZ-NH1	-6.01	117.29	120.30
1	D	96	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	E	109	LEU	CA-CB-CG	5.73	128.48	115.30
1	G	99	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	C	123	CYS	CA-CB-SG	-5.46	104.17	114.00
1	B	123	CYS	CA-CB-SG	-5.44	104.20	114.00
1	F	101	ARG	CB-CG-CD	-5.40	97.57	111.60
1	B	101	ARG	CG-CD-NE	5.31	122.95	111.80
1	F	169	ILE	C-N-CA	-5.11	108.93	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	170	PHE	Peptide
1	G	99	TYR	Sidechain

5.2 Too-close contacts

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	1125	0	1115	37	0
1	B	1103	0	1090	25	0
1	C	1150	0	1144	31	0
1	D	1106	0	1091	25	1
1	E	1118	0	1108	36	0
1	F	1139	0	1131	31	1
1	G	1125	0	1115	34	0
1	H	1130	0	1119	22	0
1	I	1125	0	1115	23	0
2	J	28	0	25	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	14	0	13	0	0
3	E	14	0	13	0	0
3	F	14	0	13	1	0
3	G	14	0	13	1	0
3	H	14	0	13	0	0
4	A	29	0	44	1	0
4	C	58	0	88	9	0
4	E	29	0	44	3	0
4	I	29	0	43	6	0
5	A	15	0	0	0	0
5	C	10	0	0	0	0
5	E	5	0	0	0	0
5	F	20	0	0	2	0
5	G	5	0	0	0	0
5	H	15	0	0	0	0
5	I	10	0	0	0	0
All	All	10486	0	10376	253	1

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 12.

All (253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LYS:HE2	1:D:167:GLU:OE2	1.63	0.97
1:B:69:ARG:HH12	1:B:173:ARG:HA	1.38	0.88
4:C:302:ERG:H263	4:C:302:ERG:H22	1.60	0.84
1:E:63:ASP:HB2	1:E:74:THR:HB	1.64	0.80
1:B:155:THR:HG22	1:B:159:ASP:H	1.47	0.79
4:C:305:ERG:H183	4:C:305:ERG:H212	1.63	0.79
1:F:63:ASP:HB2	1:F:74:THR:HB	1.64	0.79
1:F:91:ILE:HD11	1:F:109:LEU:HD13	1.65	0.79
1:A:146:LYS:HE3	1:A:167:GLU:OE2	1.86	0.74
1:A:63:ASP:HB2	1:A:74:THR:HB	1.68	0.74
1:D:155:THR:HG22	1:D:159:ASP:H	1.53	0.74
1:B:52:LYS:HG3	1:C:130:TYR:CZ	2.23	0.73
1:A:41:GLU:OE1	1:A:65:ASN:ND2	2.22	0.73
1:D:63:ASP:HB2	1:D:74:THR:HB	1.71	0.73
1:C:63:ASP:HB2	1:C:74:THR:HB	1.71	0.72
1:A:155:THR:HG22	1:A:159:ASP:H	1.52	0.72
1:B:64:PRO:HD2	1:B:73:LEU:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASN:HB3	1:A:66:PRO:HD3	1.71	0.71
1:G:155:THR:HG22	1:G:159:ASP:H	1.56	0.70
1:H:155:THR:HG22	1:H:159:ASP:H	1.55	0.70
1:B:63:ASP:HB3	1:B:64:PRO:HD3	1.74	0.70
1:E:41:GLU:OE1	1:E:65:ASN:ND2	2.25	0.69
1:E:157:LYS:HE3	1:E:159:ASP:OD2	1.92	0.69
1:E:63:ASP:HB3	1:E:64:PRO:HD3	1.75	0.68
1:G:65:ASN:HB3	1:G:66:PRO:HD3	1.75	0.68
1:H:64:PRO:HD2	1:H:73:LEU:HD12	1.74	0.68
1:H:65:ASN:HB3	1:H:66:PRO:HD3	1.75	0.68
1:G:146:LYS:HE2	1:G:167:GLU:OE2	1.95	0.66
1:I:64:PRO:HD2	1:I:73:LEU:HD12	1.78	0.65
1:A:95:VAL:HG11	4:A:302:ERG:H151	1.75	0.65
1:I:63:ASP:HB2	1:I:74:THR:HB	1.79	0.65
1:A:31:PRO:HG2	1:A:45:TYR:CZ	2.32	0.65
1:C:155:THR:HG23	1:C:157:LYS:HG3	1.78	0.64
1:C:173:ARG:HA	4:C:305:ERG:H41	1.79	0.64
1:C:155:THR:HG22	1:C:159:ASP:H	1.63	0.63
1:C:157:LYS:HE3	1:C:159:ASP:OD2	1.97	0.63
1:E:65:ASN:HB3	1:E:66:PRO:HD3	1.80	0.63
1:C:63:ASP:HB3	1:C:64:PRO:HD3	1.80	0.63
1:G:64:PRO:HD2	1:G:73:LEU:HD12	1.81	0.63
1:G:52:LYS:HG3	1:I:130:TYR:CZ	2.32	0.63
1:I:65:ASN:HB3	1:I:66:PRO:HD3	1.80	0.62
1:D:65:ASN:HB3	1:D:66:PRO:HD3	1.81	0.62
1:I:63:ASP:HB3	1:I:64:PRO:HD3	1.82	0.62
1:G:130:TYR:CZ	1:H:52:LYS:HG3	2.35	0.62
1:C:123:CYS:O	1:C:125:ILE:HG13	2.00	0.61
1:G:69:ARG:HH12	1:G:174:LEU:H	1.48	0.61
1:E:139:PRO:HG2	1:E:142:VAL:HG23	1.83	0.61
1:G:63:ASP:HB3	1:G:64:PRO:HD3	1.83	0.61
1:A:123:CYS:O	1:A:125:ILE:HG13	2.00	0.61
1:A:130:TYR:CZ	1:C:52:LYS:HG3	2.35	0.61
1:E:147:TYR:CE2	4:E:302:ERG:H7	2.35	0.61
1:B:150:VAL:HG22	1:B:165:THR:HG23	1.81	0.60
1:I:146:LYS:HE3	1:I:167:GLU:OE2	2.01	0.60
4:C:305:ERG:H212	4:C:305:ERG:C18	2.30	0.60
1:G:131:ASN:HB2	1:H:49:ILE:O	2.02	0.60
1:F:73:LEU:HD22	1:F:138:ILE:HD11	1.84	0.59
1:H:63:ASP:HB3	1:H:64:PRO:HD3	1.84	0.59
1:F:150:VAL:HG22	1:F:165:THR:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:ASP:HB2	1:H:74:THR:HB	1.84	0.59
1:F:63:ASP:HB3	1:F:64:PRO:HD3	1.84	0.58
1:D:42:SER:HB2	1:D:62:LEU:HD13	1.84	0.58
1:G:144:PRO:HD3	1:G:174:LEU:HG	1.84	0.58
1:C:91:ILE:HD11	1:C:109:LEU:HD23	1.85	0.58
1:G:123:CYS:O	1:G:125:ILE:HG13	2.04	0.58
1:C:174:LEU:HG	4:C:305:ERG:H42	1.85	0.58
1:E:130:TYR:CZ	1:F:52:LYS:HG3	2.38	0.58
1:C:150:VAL:HG22	1:C:165:THR:HG23	1.86	0.57
1:E:64:PRO:HD2	1:E:73:LEU:HD12	1.87	0.57
1:H:130:TYR:CZ	1:I:52:LYS:HG3	2.40	0.56
1:D:80:GLU:HB3	1:E:82:PHE:HE2	1.71	0.56
1:C:155:THR:CG2	1:C:157:LYS:HG3	2.35	0.56
1:A:31:PRO:HG2	1:A:45:TYR:CE2	2.41	0.56
1:A:150:VAL:HG22	1:A:165:THR:HG23	1.88	0.56
1:G:72:ASN:HD22	3:G:301:NAG:H83	1.70	0.56
1:B:63:ASP:HB2	1:B:74:THR:HB	1.88	0.55
1:G:63:ASP:HB2	1:G:74:THR:HB	1.88	0.55
1:G:146:LYS:HG2	1:G:169:ILE:HG12	1.87	0.55
1:E:73:LEU:HD22	1:E:138:ILE:HD11	1.88	0.55
4:I:304:ERG:H183	4:I:304:ERG:H212	1.88	0.55
1:H:123:CYS:O	1:H:125:ILE:HG13	2.08	0.54
1:G:41:GLU:OE1	1:G:65:ASN:ND2	2.41	0.54
1:A:155:THR:HG22	1:A:159:ASP:N	2.21	0.54
1:I:73:LEU:HD22	1:I:138:ILE:HD11	1.90	0.54
1:D:131:ASN:HB2	1:E:49:ILE:O	2.07	0.53
1:A:32:PRO:HB2	1:A:33:PRO:HD2	1.89	0.53
4:I:304:ERG:H211	4:I:304:ERG:H263	1.88	0.53
1:B:91:ILE:HD11	1:B:109:LEU:HD13	1.89	0.53
1:F:146:LYS:HG2	1:F:169:ILE:HD12	1.90	0.53
1:H:155:THR:HG23	1:H:157:LYS:H	1.73	0.53
1:E:155:THR:HG22	1:E:159:ASP:H	1.74	0.53
1:A:87:GLU:HA	1:A:110:CYS:SG	2.49	0.52
1:C:126:GLU:HG2	1:F:71:GLU:OE2	2.09	0.52
1:I:147:TYR:CD2	4:I:304:ERG:H7	2.44	0.52
1:D:155:THR:HG22	1:D:159:ASP:N	2.24	0.52
4:I:304:ERG:H263	4:I:304:ERG:C21	2.40	0.52
1:G:155:THR:HG22	1:G:159:ASP:N	2.24	0.52
1:F:72:ASN:OD1	1:F:137:GLU:HG2	2.10	0.52
1:A:73:LEU:HD22	1:A:138:ILE:HD11	1.91	0.52
1:D:64:PRO:HD2	1:D:73:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:VAL:HG22	1:G:165:THR:HG23	1.92	0.52
1:G:99:TYR:CD1	1:G:99:TYR:C	2.83	0.51
1:A:81:VAL:O	1:A:127:PRO:HA	2.09	0.51
1:C:58:LYS:NZ	1:C:80:GLU:OE1	2.43	0.51
1:D:52:LYS:HD3	1:F:130:TYR:OH	2.09	0.51
1:E:96:ARG:NH1	1:E:98:GLY:O	2.41	0.51
1:D:91:ILE:HD11	1:D:109:LEU:HD13	1.93	0.51
1:F:152:ARG:HB3	1:F:154:TYR:HE1	1.76	0.51
1:G:99:TYR:C	1:G:99:TYR:HD1	2.15	0.51
1:A:69:ARG:NH2	1:A:142:VAL:O	2.38	0.50
1:B:155:THR:HG22	1:B:159:ASP:N	2.21	0.50
1:F:99:TYR:CD1	1:F:100:ILE:HG13	2.46	0.50
1:H:91:ILE:HD11	1:H:109:LEU:HD23	1.93	0.50
1:B:69:ARG:NH1	1:B:173:ARG:HA	2.17	0.50
1:H:146:LYS:HE3	1:H:167:GLU:OE2	2.12	0.50
1:E:150:VAL:HG22	1:E:165:THR:HG23	1.94	0.50
1:F:155:THR:HG22	1:F:159:ASP:H	1.76	0.50
1:D:97:LEU:HD23	1:D:147:TYR:CD1	2.47	0.50
1:D:155:THR:HG23	1:D:157:LYS:H	1.76	0.50
1:A:49:ILE:O	1:B:131:ASN:HB2	2.12	0.49
1:C:155:THR:HG22	1:C:159:ASP:N	2.25	0.49
1:A:52:LYS:HD2	1:B:130:TYR:OH	2.12	0.49
4:C:305:ERG:H161	1:G:95:VAL:HG11	1.95	0.49
1:A:123:CYS:O	1:A:125:ILE:N	2.45	0.49
1:B:94:GLU:OE2	1:B:101:ARG:HD3	2.13	0.49
1:E:110:CYS:HB3	1:E:123:CYS:HB2	1.67	0.49
1:C:94:GLU:OE2	1:C:96:ARG:NH2	2.39	0.49
1:E:147:TYR:CD2	4:E:302:ERG:H7	2.47	0.49
1:F:91:ILE:HD11	1:F:109:LEU:CD1	2.39	0.49
1:H:155:THR:HG22	1:H:159:ASP:N	2.25	0.49
1:C:110:CYS:HB3	1:C:123:CYS:HB2	1.57	0.48
1:D:110:CYS:HB3	1:D:123:CYS:HB2	1.54	0.48
1:G:108:ASP:HB3	1:G:111:GLU:HB3	1.96	0.48
1:I:44:LEU:HD12	1:I:60:VAL:HG11	1.96	0.48
1:I:91:ILE:HD11	1:I:109:LEU:HD13	1.94	0.48
1:G:73:LEU:HD22	1:G:138:ILE:HD11	1.96	0.47
1:H:44:LEU:HD12	1:H:60:VAL:HG11	1.96	0.47
1:B:65:ASN:HB3	1:B:66:PRO:CD	2.44	0.47
1:F:99:TYR:CD1	1:F:99:TYR:C	2.87	0.47
1:E:152:ARG:HB3	1:E:154:TYR:HE1	1.78	0.47
4:C:305:ERG:C19	4:C:305:ERG:H182	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:ILE:HG22	1:H:102:LEU:HD12	1.97	0.47
1:B:73:LEU:HD22	1:B:138:ILE:HD11	1.97	0.47
1:C:57:ILE:HD13	1:C:164:LEU:HD11	1.97	0.47
1:E:157:LYS:O	1:E:158:ASP:HB2	2.14	0.47
1:H:41:GLU:OE1	1:H:65:ASN:ND2	2.48	0.47
1:I:147:TYR:CE2	4:I:304:ERG:H7	2.49	0.47
1:A:84:THR:HG21	1:F:175:VAL:HG22	1.97	0.47
1:F:169:ILE:HG22	1:F:170:PHE:O	2.15	0.47
1:G:49:ILE:O	1:I:131:ASN:HB2	2.15	0.47
1:C:101:ARG:HD3	1:C:104:SER:HB2	1.96	0.47
1:D:123:CYS:O	1:D:125:ILE:HG13	2.15	0.46
1:D:150:VAL:HG22	1:D:165:THR:HG23	1.96	0.46
1:E:63:ASP:HB3	1:E:64:PRO:CD	2.44	0.46
1:G:35:THR:HA	1:G:46:GLN:O	2.15	0.46
1:G:47:CYS:O	1:G:163:CYS:HB3	2.15	0.46
1:A:171:PRO:HA	1:A:172:PRO:HD3	1.83	0.46
1:F:152:ARG:HB3	1:F:154:TYR:CE1	2.50	0.46
1:G:146:LYS:CE	1:G:167:GLU:OE2	2.61	0.46
1:A:105:GLN:HG3	1:A:107:PHE:CE1	2.51	0.46
1:A:124:PRO:HB3	1:F:175:VAL:HG21	1.97	0.46
1:E:152:ARG:HB3	1:E:154:TYR:CE1	2.51	0.46
1:F:64:PRO:HD2	1:F:73:LEU:HD12	1.98	0.46
1:F:99:TYR:C	1:F:99:TYR:HD1	2.19	0.46
4:E:302:ERG:H263	4:E:302:ERG:C21	2.47	0.45
1:H:73:LEU:HD22	1:H:138:ILE:HD11	1.98	0.45
1:C:64:PRO:HD2	1:C:73:LEU:HD12	1.98	0.45
1:G:123:CYS:O	1:G:125:ILE:N	2.49	0.45
1:A:121:LEU:HD11	1:A:132:ILE:HD11	1.98	0.45
1:E:58:LYS:HD2	1:E:80:GLU:OE2	2.17	0.45
1:G:144:PRO:CD	1:G:174:LEU:HG	2.47	0.45
1:F:110:CYS:HB3	1:F:123:CYS:HB2	1.81	0.45
1:C:152:ARG:HB3	1:C:154:TYR:CE1	2.51	0.45
1:A:52:LYS:HD2	1:B:130:TYR:CZ	2.52	0.45
1:I:126:GLU:O	1:I:130:TYR:OH	2.22	0.45
1:A:64:PRO:HD2	1:A:73:LEU:HD12	1.99	0.45
1:B:83:GLU:OE2	1:C:126:GLU:HB3	2.17	0.45
1:I:150:VAL:HG22	1:I:165:THR:HG23	1.98	0.45
1:F:146:LYS:HG2	1:F:169:ILE:CD1	2.46	0.45
1:B:110:CYS:HB3	1:B:123:CYS:HB2	1.76	0.44
3:F:301:NAG:H82	5:F:305:SO4:O4	2.17	0.44
4:C:305:ERG:H282	4:C:305:ERG:H211	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:ASN:ND2	5:F:304:SO4:O2	2.44	0.44
1:F:55:VAL:HG22	1:F:81:VAL:HG22	1.99	0.44
1:I:123:CYS:O	1:I:125:ILE:HG13	2.17	0.44
1:E:119:GLU:O	1:E:121:LEU:HD13	2.18	0.44
1:H:123:CYS:O	1:H:125:ILE:N	2.50	0.44
1:C:58:LYS:NZ	1:C:58:LYS:HB2	2.33	0.44
1:H:155:THR:HG23	1:H:157:LYS:N	2.33	0.44
1:I:97:LEU:HD13	1:I:147:TYR:CE1	2.53	0.44
1:B:123:CYS:O	1:B:125:ILE:HG13	2.18	0.44
1:E:82:PHE:N	1:E:82:PHE:CD1	2.86	0.43
1:H:110:CYS:HB3	1:H:123:CYS:HB2	1.76	0.43
1:C:175:VAL:HG12	1:C:177:ARG:HG3	2.00	0.43
1:E:78:ASN:OD1	1:F:36:LYS:HE3	2.19	0.43
1:G:97:LEU:HD13	1:G:147:TYR:CE1	2.53	0.43
1:I:155:THR:HG22	1:I:159:ASP:H	1.83	0.43
1:E:55:VAL:HG22	1:E:81:VAL:HG22	2.00	0.43
1:I:147:TYR:CD2	4:I:304:ERG:H151	2.53	0.43
1:F:80:GLU:OE2	1:F:129:GLU:OE1	2.37	0.43
1:A:102:LEU:HD12	1:A:102:LEU:HA	1.70	0.43
1:D:63:ASP:HB3	1:D:64:PRO:CD	2.49	0.43
1:G:110:CYS:HB3	1:G:123:CYS:HB2	1.64	0.43
1:D:97:LEU:HD23	1:D:147:TYR:CE1	2.54	0.43
1:A:91:ILE:CG1	1:A:109:LEU:HD23	2.49	0.43
1:B:44:LEU:HD12	1:B:60:VAL:HG11	2.01	0.43
1:D:69:ARG:HB3	1:D:140:GLY:HA2	2.00	0.43
1:D:130:TYR:CZ	1:E:52:LYS:HG3	2.54	0.43
1:H:152:ARG:HB3	1:H:154:TYR:CE1	2.54	0.43
1:F:81:VAL:O	1:F:127:PRO:HA	2.18	0.42
1:H:62:LEU:HD23	1:H:67:PRO:HG3	2.01	0.42
1:E:155:THR:HG22	1:E:159:ASP:N	2.34	0.42
1:C:97:LEU:HB2	1:C:102:LEU:HD11	2.00	0.42
1:D:154:TYR:N	1:D:154:TYR:CD1	2.87	0.42
1:E:82:PHE:N	1:E:82:PHE:HD1	2.16	0.42
1:B:143:PRO:HG2	1:B:147:TYR:OH	2.19	0.42
1:A:63:ASP:HB3	1:A:64:PRO:CD	2.49	0.42
1:E:81:VAL:O	1:E:127:PRO:HA	2.20	0.42
1:D:61:ASN:HB2	1:D:76:SER:HB2	2.01	0.42
1:E:44:LEU:HD12	1:E:60:VAL:HG11	2.02	0.42
1:E:51:ASP:O	1:E:53:GLN:HG3	2.20	0.42
1:B:91:ILE:HD11	1:B:109:LEU:CD1	2.49	0.42
1:B:119:GLU:OE1	1:B:119:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:LEU:CD1	1:C:118:ILE:HB	2.50	0.42
1:G:51:ASP:O	1:G:53:GLN:HG3	2.19	0.42
1:E:44:LEU:HA	1:E:44:LEU:HD23	1.84	0.41
1:B:35:THR:HA	1:B:46:GLN:O	2.20	0.41
1:B:152:ARG:HB3	1:B:154:TYR:CE1	2.54	0.41
1:D:113:LEU:HD13	1:D:121:LEU:HB3	2.03	0.41
1:E:76:SER:HA	1:E:132:ILE:O	2.20	0.41
1:C:91:ILE:HD11	1:C:109:LEU:CD2	2.50	0.41
1:A:67:PRO:HB3	1:A:138:ILE:CD1	2.51	0.41
1:A:31:PRO:HB2	1:A:35:THR:HG21	2.03	0.41
1:C:63:ASP:HB3	1:C:64:PRO:CD	2.50	0.41
4:C:305:ERG:H162	1:G:147:TYR:CD2	2.55	0.41
1:D:155:THR:HG23	1:D:157:LYS:N	2.35	0.41
1:A:91:ILE:HD11	1:A:109:LEU:HD23	2.03	0.41
1:A:152:ARG:HB3	1:A:154:TYR:CE1	2.55	0.41
1:C:165:THR:HG22	1:C:166:GLY:N	2.35	0.41
1:G:81:VAL:O	1:G:127:PRO:HA	2.20	0.41
1:I:35:THR:HA	1:I:46:GLN:O	2.21	0.41
1:A:139:PRO:HG2	1:A:142:VAL:CG2	2.51	0.41
1:E:64:PRO:HD2	1:E:73:LEU:CD1	2.51	0.41
1:F:82:PHE:HD1	1:F:82:PHE:N	2.19	0.41
1:I:110:CYS:HB3	1:I:123:CYS:HB2	1.70	0.40
1:I:152:ARG:HB3	1:I:154:TYR:CE1	2.56	0.40
1:C:123:CYS:O	1:C:125:ILE:N	2.54	0.40
1:D:142:VAL:HA	1:D:143:PRO:HD3	1.91	0.40
1:E:97:LEU:HD13	1:E:147:TYR:CZ	2.57	0.40
1:F:103:LEU:HD11	1:F:105:GLN:HG2	2.03	0.40
1:G:83:GLU:OE2	1:I:126:GLU:HB3	2.21	0.40
1:A:47:CYS:O	1:A:163:CYS:HB3	2.22	0.40
1:A:110:CYS:HB3	1:A:123:CYS:HB2	1.92	0.40
1:F:82:PHE:N	1:F:82:PHE:CD1	2.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:TYR:O	1:F:101:ARG:NH1[6_555]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	142/201 (71%)	138 (97%)	4 (3%)	0	100	100
1	B	139/201 (69%)	134 (96%)	5 (4%)	0	100	100
1	C	145/201 (72%)	141 (97%)	4 (3%)	0	100	100
1	D	140/201 (70%)	137 (98%)	3 (2%)	0	100	100
1	E	141/201 (70%)	135 (96%)	6 (4%)	0	100	100
1	F	144/201 (72%)	140 (97%)	3 (2%)	1 (1%)	19	49
1	G	142/201 (71%)	136 (96%)	6 (4%)	0	100	100
1	H	143/201 (71%)	140 (98%)	3 (2%)	0	100	100
1	I	142/201 (71%)	138 (97%)	4 (3%)	0	100	100
All	All	1278/1809 (71%)	1239 (97%)	38 (3%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	171	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/168 (77%)	125 (96%)	5 (4%)	28	63
1	B	127/168 (76%)	118 (93%)	9 (7%)	12	36
1	C	133/168 (79%)	129 (97%)	4 (3%)	36	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	128/168 (76%)	122 (95%)	6 (5%)	22	55
1	E	129/168 (77%)	122 (95%)	7 (5%)	18	49
1	F	132/168 (79%)	127 (96%)	5 (4%)	28	63
1	G	130/168 (77%)	122 (94%)	8 (6%)	15	43
1	H	130/168 (77%)	124 (95%)	6 (5%)	23	55
1	I	130/168 (77%)	126 (97%)	4 (3%)	35	70
All	All	1169/1512 (77%)	1115 (95%)	54 (5%)	23	55

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	TYR
1	A	130	TYR
1	A	147	TYR
1	A	154	TYR
1	A	157	LYS
1	B	46	GLN
1	B	52	LYS
1	B	101	ARG
1	B	119	GLU
1	B	130	TYR
1	B	137	GLU
1	B	147	TYR
1	B	154	TYR
1	B	173	ARG
1	C	52	LYS
1	C	130	TYR
1	C	154	TYR
1	C	157	LYS
1	D	78	ASN
1	D	82	PHE
1	D	109	LEU
1	D	130	TYR
1	D	147	TYR
1	D	154	TYR
1	E	52	LYS
1	E	78	ASN
1	E	82	PHE
1	E	100	ILE
1	E	130	TYR

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Mol	Chain	Res	Type
1	E	147	TYR
1	E	154	TYR
1	F	99	TYR
1	F	113	LEU
1	F	130	TYR
1	F	147	TYR
1	F	154	TYR
1	G	45	TYR
1	G	52	LYS
1	G	82	PHE
1	G	99	TYR
1	G	130	TYR
1	G	147	TYR
1	G	154	TYR
1	G	174	LEU
1	H	45	TYR
1	H	52	LYS
1	H	82	PHE
1	H	130	TYR
1	H	147	TYR
1	H	154	TYR
1	I	45	TYR
1	I	130	TYR
1	I	147	TYR
1	I	154	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	C	46	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

2 monosaccharides 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	NAG	J	1	2,1	14,14,15	0.33	0	17,19,21	0.80	1 (5%)
2	NAG	J	2	2	14,14,15	0.30	0	17,19,21	0.71	1 (5%)

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	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	NAG	C1-O5-C5	2.71	115.86	112.19
2	J	2	NAG	C1-O5-C5	2.37	115.40	112.19

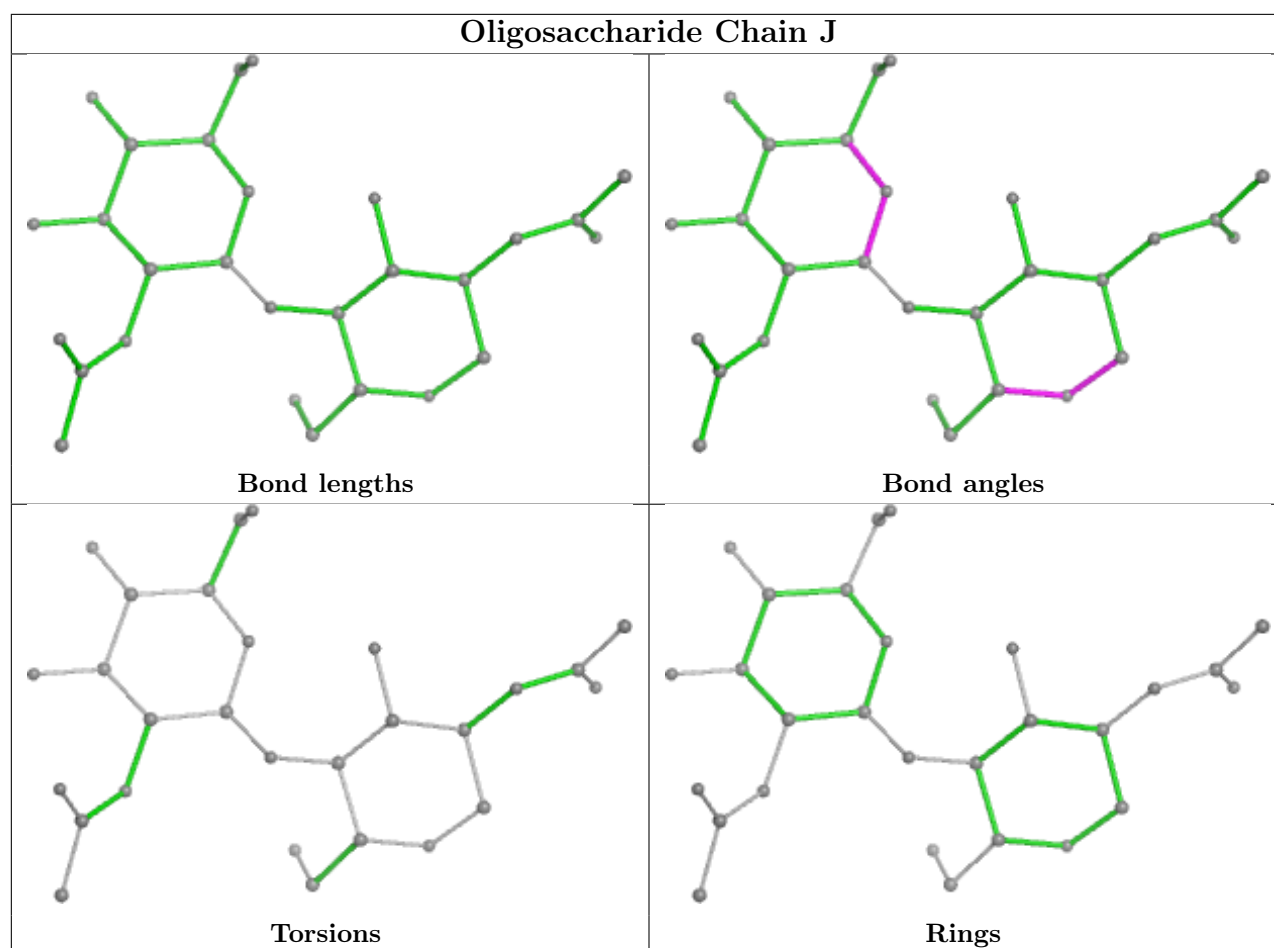
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

29 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	$\# Z > 2$
3	NAG	E	301	1	14,14,15	0.67	0	17,19,21	0.46	0
4	ERG	C	302	-	31,32,32	0.18	0	47,50,50	0.47	0
5	SO4	H	304	-	4,4,4	0.13	0	6,6,6	0.19	0
3	NAG	H	301	1	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
3	NAG	F	301	1	14,14,15	0.38	0	17,19,21	0.64	1 (5%)
5	SO4	H	302	-	4,4,4	0.16	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	E	303	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	C	304	-	4,4,4	0.15	0	6,6,6	0.11	0
5	SO4	A	304	-	4,4,4	0.20	0	6,6,6	0.44	0
5	SO4	I	303	-	4,4,4	0.15	0	6,6,6	0.26	0
4	ERG	E	302	-	31,32,32	0.19	0	47,50,50	0.50	0
4	ERG	C	305	-	31,32,32	0.49	0	47,50,50	1.20	3 (6%)
5	SO4	A	305	-	4,4,4	0.12	0	6,6,6	0.33	0
5	SO4	G	302	-	4,4,4	0.12	0	6,6,6	0.17	0
4	ERG	I	304	-	31,32,32	0.35	0	47,50,50	1.07	4 (8%)
5	SO4	I	305	-	4,4,4	0.13	0	6,6,6	0.17	0
5	SO4	F	304	-	4,4,4	0.15	0	6,6,6	0.20	0
3	NAG	A	301	1	14,14,15	0.47	0	17,19,21	0.59	0
3	NAG	B	301	1	14,14,15	0.47	0	17,19,21	0.54	0
5	SO4	F	302	-	4,4,4	0.11	0	6,6,6	0.16	0
5	SO4	H	303	-	4,4,4	0.12	0	6,6,6	0.17	0
3	NAG	C	301	1	14,14,15	0.43	0	17,19,21	0.49	0
5	SO4	F	305	-	4,4,4	0.17	0	6,6,6	0.15	0
5	SO4	A	303	-	4,4,4	0.15	0	6,6,6	0.21	0
5	SO4	F	303	-	4,4,4	0.13	0	6,6,6	0.12	0
5	SO4	C	303	-	4,4,4	0.15	0	6,6,6	0.12	0
4	ERG	A	302	-	31,32,32	0.21	0	47,50,50	0.47	0
3	NAG	D	301	1	14,14,15	0.62	0	17,19,21	0.70	1 (5%)
3	NAG	G	301	1	14,14,15	0.34	0	17,19,21	0.52	0

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	NAG	E	301	1	-	1/6/23/26	0/1/1/1
4	ERG	C	302	-	-	3/13/71/71	0/4/4/4
4	ERG	I	304	-	-	8/13/71/71	0/4/4/4
3	NAG	H	301	1	-	1/6/23/26	0/1/1/1
4	ERG	E	302	-	-	8/13/71/71	0/4/4/4
3	NAG	F	301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	301	1	-	2/6/23/26	0/1/1/1
4	ERG	C	305	-	-	11/13/71/71	0/4/4/4
4	ERG	A	302	-	-	5/13/71/71	0/4/4/4
3	NAG	B	301	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	301	1	-	2/6/23/26	0/1/1/1
3	NAG	G	301	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	305	ERG	C16-C15-C14	-4.10	98.55	105.30
3	H	301	NAG	C1-O5-C5	3.43	116.85	112.19
4	C	305	ERG	C21-C20-C22	-3.04	102.64	109.99
4	I	304	ERG	C13-C14-C8	2.91	119.13	113.48
4	C	305	ERG	C11-C9-C8	2.90	117.83	111.33
4	I	304	ERG	C14-C13-C17	-2.53	97.02	99.72
3	D	301	NAG	C1-O5-C5	2.50	115.58	112.19
3	F	301	NAG	C1-O5-C5	2.18	115.15	112.19
4	I	304	ERG	C16-C15-C14	-2.18	101.71	105.30
4	I	304	ERG	C11-C9-C8	2.15	116.13	111.33

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	302	ERG	C22-C23-C24-C25
4	C	305	ERG	C13-C17-C20-C21
4	C	305	ERG	C20-C22-C23-C24
4	C	305	ERG	C23-C24-C25-C26
4	C	305	ERG	C23-C24-C25-C27
4	C	305	ERG	C28-C24-C25-C26
4	C	305	ERG	C28-C24-C25-C27
4	E	302	ERG	C20-C22-C23-C24
4	I	304	ERG	C13-C17-C20-C21
4	I	304	ERG	C16-C17-C20-C21
4	I	304	ERG	C16-C17-C20-C22
4	I	304	ERG	C20-C22-C23-C24
4	I	304	ERG	C22-C23-C24-C25
3	F	301	NAG	C4-C5-C6-O6
3	A	301	NAG	O5-C5-C6-O6
3	F	301	NAG	O5-C5-C6-O6
3	G	301	NAG	C8-C7-N2-C2
3	G	301	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	A	301	NAG	C4-C5-C6-O6
3	B	301	NAG	O5-C5-C6-O6
4	C	302	ERG	C17-C20-C22-C23
4	E	302	ERG	C17-C20-C22-C23
3	G	301	NAG	O5-C5-C6-O6
3	C	301	NAG	O5-C5-C6-O6
4	I	304	ERG	C22-C23-C24-C28
4	A	302	ERG	C20-C22-C23-C24
3	B	301	NAG	C4-C5-C6-O6
3	C	301	NAG	C4-C5-C6-O6
4	C	305	ERG	C13-C17-C20-C22
4	C	305	ERG	C16-C17-C20-C22
4	I	304	ERG	C13-C17-C20-C22
4	A	302	ERG	C22-C23-C24-C25
4	C	302	ERG	C21-C20-C22-C23
4	E	302	ERG	C21-C20-C22-C23
4	C	305	ERG	C21-C20-C22-C23
4	E	302	ERG	C22-C23-C24-C28
3	E	301	NAG	O5-C5-C6-O6
4	E	302	ERG	C23-C24-C25-C26
4	I	304	ERG	C17-C20-C22-C23
4	A	302	ERG	C28-C24-C25-C26
4	C	305	ERG	C16-C17-C20-C21
4	E	302	ERG	C22-C23-C24-C25
4	E	302	ERG	C28-C24-C25-C26
3	H	301	NAG	C3-C2-N2-C7
4	A	302	ERG	C23-C24-C25-C26
4	C	305	ERG	C17-C20-C22-C23
4	A	302	ERG	C22-C23-C24-C28
4	E	302	ERG	C28-C24-C25-C27

There are no ring outliers.

9 monomers are involved in 22 short contacts:

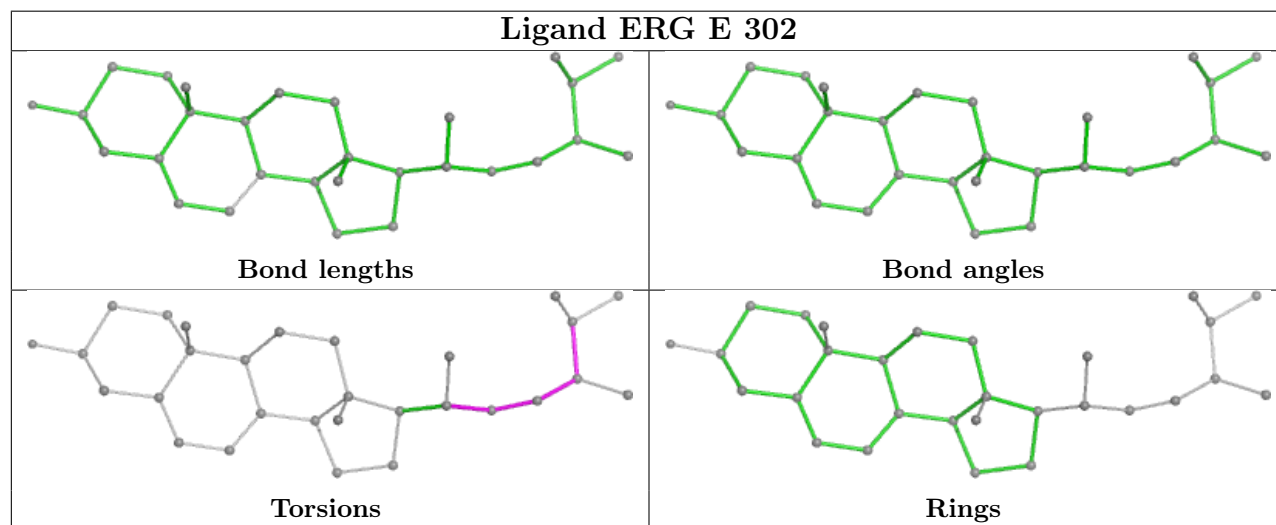
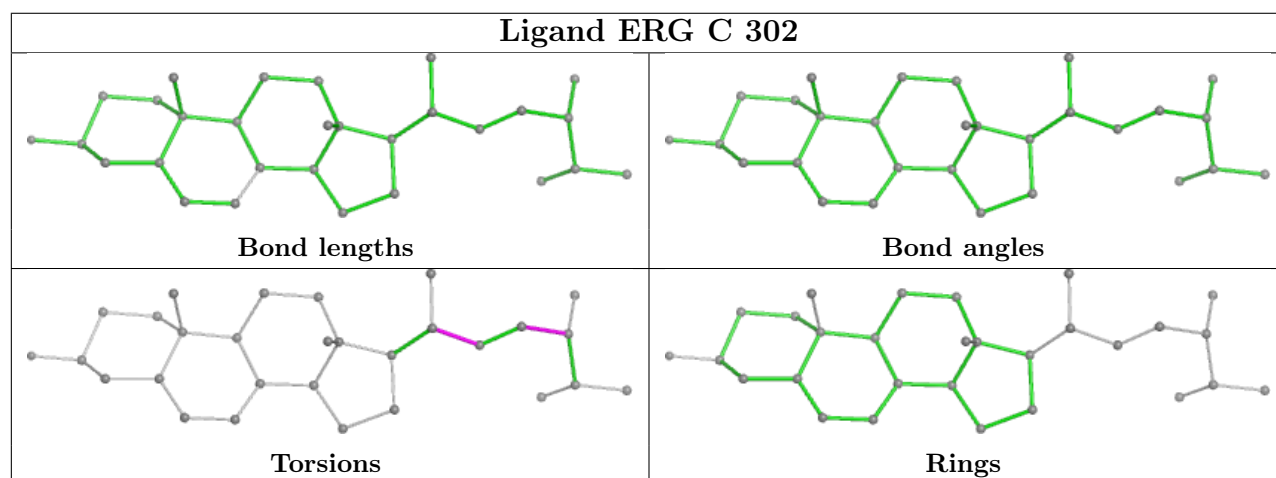
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	302	ERG	1	0
3	F	301	NAG	1	0
4	E	302	ERG	3	0
4	C	305	ERG	8	0
4	I	304	ERG	6	0
5	F	304	SO4	1	0
5	F	305	SO4	1	0

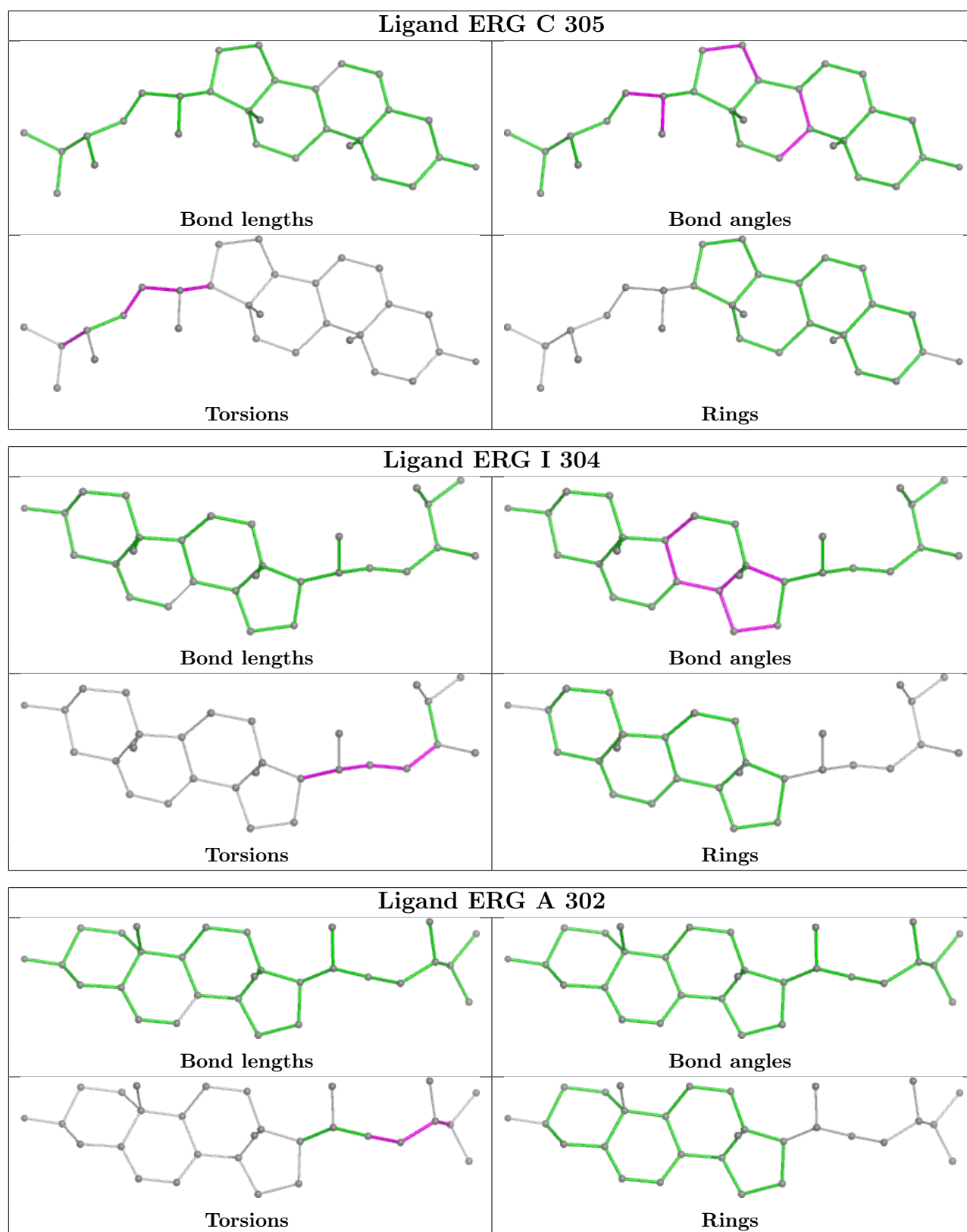
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	ERG	1	0
3	G	301	NAG	1	0

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 [i](#)

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	144/201 (71%)	0.30	15 (10%) 13 12	33, 60, 117, 147	0
1	B	141/201 (70%)	0.15	11 (7%) 20 18	28, 52, 94, 140	0
1	C	147/201 (73%)	0.00	13 (8%) 17 15	27, 49, 95, 140	0
1	D	142/201 (70%)	1.13	37 (26%) 2 2	47, 97, 152, 172	0
1	E	143/201 (71%)	0.54	17 (11%) 10 9	42, 69, 116, 161	0
1	F	146/201 (72%)	0.48	14 (9%) 15 13	33, 63, 111, 162	0
1	G	144/201 (71%)	0.16	13 (9%) 17 14	30, 52, 98, 144	0
1	H	145/201 (72%)	0.08	10 (6%) 24 20	27, 50, 96, 142	0
1	I	144/201 (71%)	0.43	12 (8%) 19 16	38, 62, 115, 137	0
All	All	1296/1809 (71%)	0.36	142 (10%) 12 10	27, 60, 123, 172	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	29	ALA	9.1
1	F	58	LYS	7.6
1	I	174	LEU	7.1
1	G	31	PRO	6.6
1	A	174	LEU	6.5
1	D	31	PRO	5.9
1	E	174	LEU	5.9
1	E	32	PRO	5.9
1	C	31	PRO	5.8
1	D	172	PRO	5.8
1	G	174	LEU	5.8
1	D	123	CYS	5.5
1	I	31	PRO	5.5
1	F	31	PRO	5.5
1	D	171	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
1	H	30	LEU	5.2
1	B	33	PRO	5.1
1	H	31	PRO	5.1
1	E	99	TYR	5.1
1	C	32	PRO	5.0
1	B	123	CYS	4.8
1	A	172	PRO	4.7
1	A	31	PRO	4.7
1	F	32	PRO	4.7
1	G	121	LEU	4.6
1	H	69	ARG	4.5
1	G	32	PRO	4.5
1	C	123	CYS	4.5
1	B	173	ARG	4.5
1	F	63	ASP	4.5
1	F	174	LEU	4.4
1	G	173	ARG	4.4
1	F	176	PRO	4.4
1	H	32	PRO	4.4
1	A	32	PRO	4.3
1	E	123	CYS	4.3
1	D	144	PRO	4.1
1	C	65	ASN	4.1
1	E	33	PRO	4.1
1	D	120	GLY	4.1
1	A	63	ASP	4.0
1	E	157	LYS	4.0
1	I	172	PRO	4.0
1	E	171	PRO	4.0
1	A	121	LEU	3.9
1	A	65	ASN	3.9
1	B	119	GLU	3.8
1	A	173	ARG	3.8
1	H	33	PRO	3.8
1	B	63	ASP	3.8
1	F	124	PRO	3.7
1	D	124	PRO	3.7
1	C	33	PRO	3.6
1	F	175	VAL	3.6
1	C	99	TYR	3.6
1	I	173	ARG	3.5
1	A	141	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	119	GLU	3.5
1	H	123	CYS	3.5
1	E	173	ARG	3.5
1	G	172	PRO	3.5
1	G	120	GLY	3.4
1	D	68	VAL	3.4
1	D	114	GLU	3.4
1	I	113	LEU	3.3
1	I	123	CYS	3.3
1	D	143	PRO	3.3
1	G	33	PRO	3.2
1	I	65	ASN	3.2
1	D	103	LEU	3.2
1	E	172	PRO	3.2
1	D	99	TYR	3.2
1	F	122	SER	3.1
1	D	118	ILE	3.1
1	G	155	THR	3.1
1	G	123	CYS	3.1
1	D	102	LEU	3.1
1	D	146	LYS	3.1
1	I	63	ASP	3.0
1	D	94	GLU	3.0
1	A	33	PRO	2.9
1	F	120	GLY	2.8
1	D	156	GLU	2.8
1	B	124	PRO	2.7
1	D	122	SER	2.7
1	F	123	CYS	2.7
1	E	114	GLU	2.7
1	B	100	ILE	2.7
1	D	100	ILE	2.7
1	A	171	PRO	2.7
1	E	119	GLU	2.6
1	I	77	ALA	2.6
1	E	124	PRO	2.6
1	F	173	ARG	2.6
1	H	65	ASN	2.5
1	D	96	ARG	2.5
1	B	118	ILE	2.5
1	B	120	GLY	2.5
1	C	63	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	177	ARG	2.5
1	C	124	PRO	2.5
1	E	121	LEU	2.5
1	D	69	ARG	2.4
1	D	140	GLY	2.4
1	A	123	CYS	2.4
1	D	133	LYS	2.4
1	D	70	GLY	2.4
1	G	119	GLU	2.4
1	D	141	GLU	2.4
1	I	141	GLU	2.4
1	E	120	GLY	2.3
1	E	156	GLU	2.3
1	H	96	ARG	2.3
1	D	65	ASN	2.3
1	D	66	PRO	2.3
1	D	170	PHE	2.3
1	G	137	GLU	2.3
1	D	121	LEU	2.3
1	A	96	ARG	2.2
1	B	156	GLU	2.2
1	C	141	GLU	2.2
1	D	137	GLU	2.2
1	F	128	GLY	2.2
1	I	137	GLU	2.2
1	B	65	ASN	2.1
1	A	119	GLU	2.1
1	G	63	ASP	2.1
1	D	169	ILE	2.1
1	I	100	ILE	2.1
1	D	101	ARG	2.1
1	F	99	TYR	2.1
1	C	122	SER	2.1
1	D	147	TYR	2.1
1	D	117	ASP	2.0
1	E	105	GLN	2.0
1	H	137	GLU	2.0
1	D	145	GLY	2.0
1	A	99	TYR	2.0
1	D	139	PRO	2.0
1	C	34	ASN	2.0
1	E	96	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	103	LEU	2.0

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

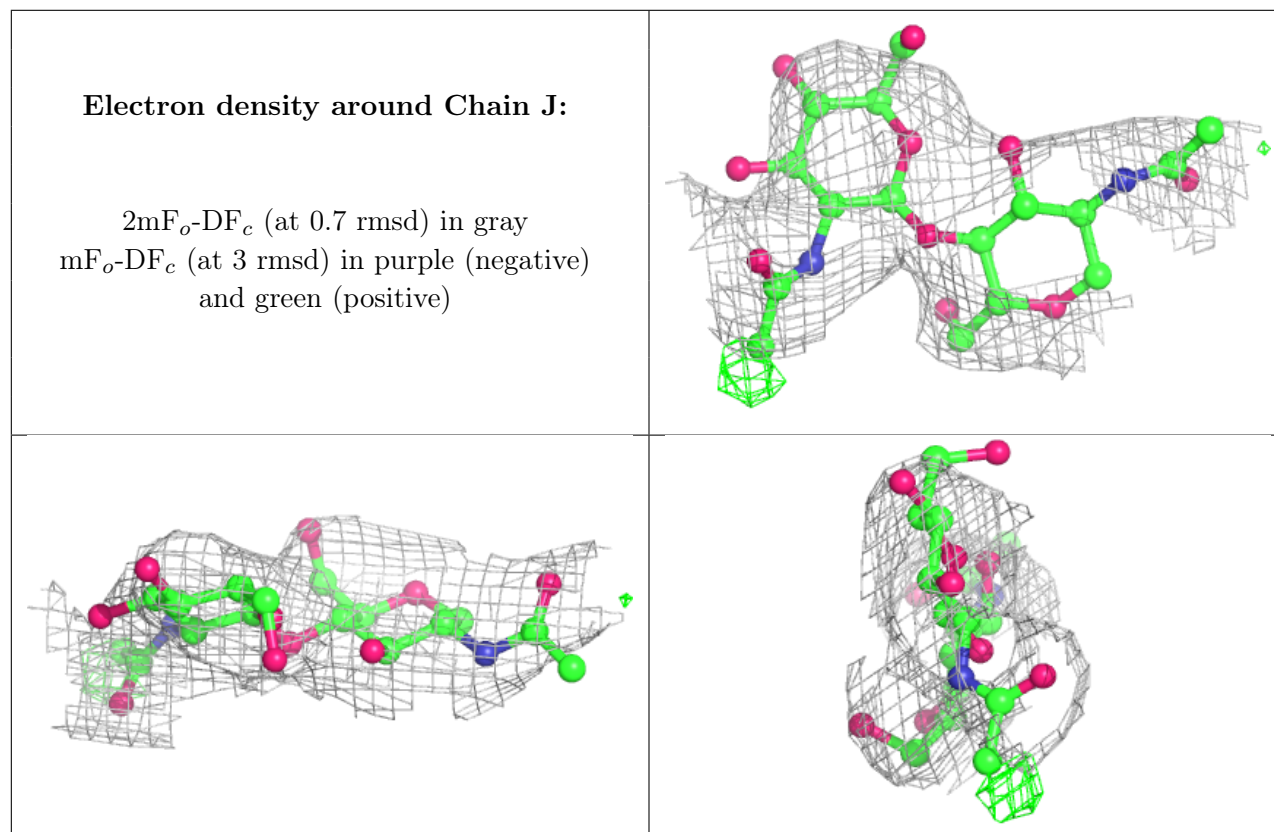
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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	NAG	J	2	14/15	0.53	0.18	131,156,158,158	0
2	NAG	J	1	14/15	0.72	0.19	121,132,141,150	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands ⓘ

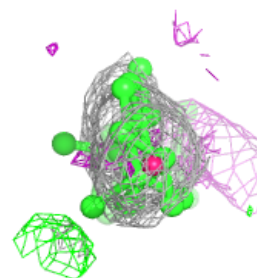
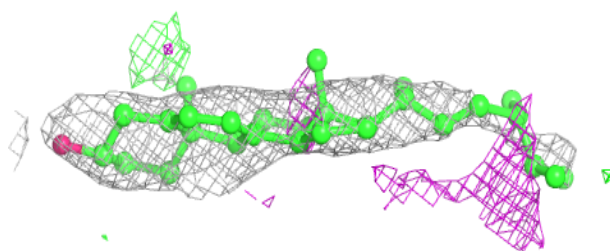
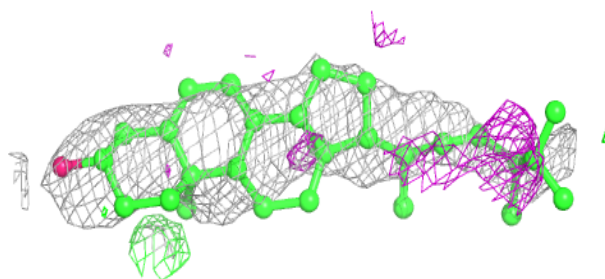
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	H	302	5/5	0.36	0.31	190,191,202,262	0
3	NAG	G	301	14/15	0.50	0.19	108,119,124,126	0
3	NAG	H	301	14/15	0.62	0.23	122,131,139,148	0
3	NAG	E	301	14/15	0.68	0.16	118,128,135,136	0
3	NAG	D	301	14/15	0.70	0.18	142,152,170,181	0
5	SO4	C	304	5/5	0.72	0.10	149,150,156,157	0
3	NAG	A	301	14/15	0.72	0.18	114,136,138,140	0
3	NAG	C	301	14/15	0.74	0.17	92,113,120,124	0
3	NAG	F	301	14/15	0.75	0.17	98,112,126,128	0
5	SO4	G	302	5/5	0.76	0.10	123,126,127,130	0
3	NAG	B	301	14/15	0.76	0.17	121,128,134,139	0
5	SO4	F	302	5/5	0.77	0.12	128,134,136,138	0
5	SO4	E	303	5/5	0.78	0.18	150,153,156,156	0
5	SO4	A	303	5/5	0.78	0.18	147,153,155,157	0
5	SO4	H	303	5/5	0.78	0.15	133,133,139,139	0
4	ERG	A	302	29/29	0.80	0.27	66,101,111,115	0
5	SO4	F	303	5/5	0.81	0.09	137,137,140,140	0
4	ERG	C	305	29/29	0.82	0.29	58,87,104,110	0
5	SO4	F	304	5/5	0.85	0.13	124,125,131,133	0
5	SO4	H	304	5/5	0.86	0.19	107,111,115,117	0
5	SO4	I	305	5/5	0.87	0.14	139,142,144,144	0
4	ERG	I	304	29/29	0.88	0.23	78,94,103,107	0
4	ERG	C	302	29/29	0.88	0.24	72,91,112,113	0
5	SO4	F	305	5/5	0.88	0.21	121,122,124,132	0
5	SO4	C	303	5/5	0.88	0.12	125,126,127,131	0
4	ERG	E	302	29/29	0.90	0.21	75,93,104,107	0
5	SO4	A	305	5/5	0.90	0.11	90,100,104,104	0
5	SO4	A	304	5/5	0.98	0.07	63,65,77,78	0
5	SO4	I	303	5/5	0.99	0.05	61,66,76,78	0

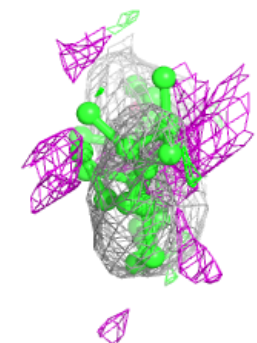
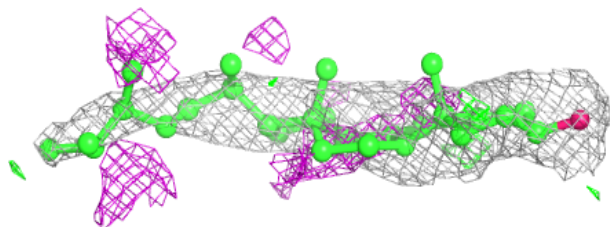
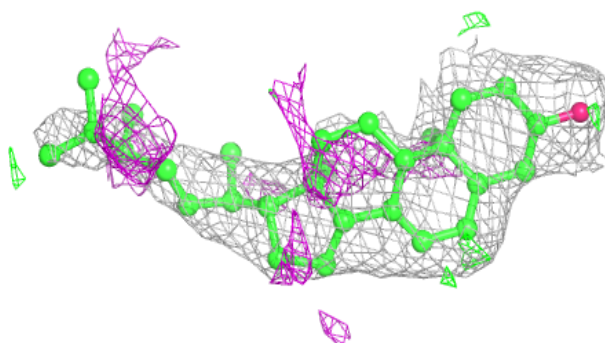
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ERG A 302:

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

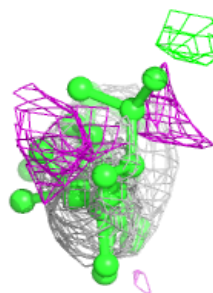
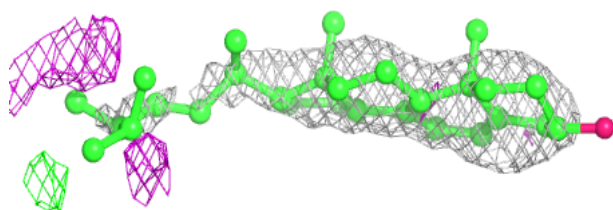
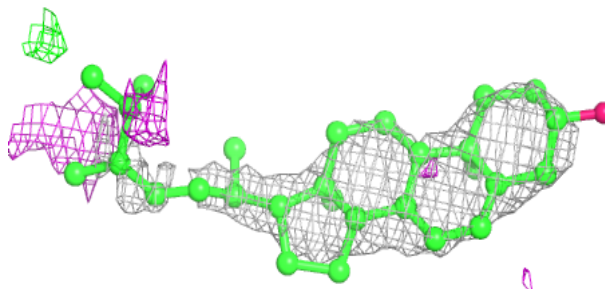
**Electron density around ERG C 305:**

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

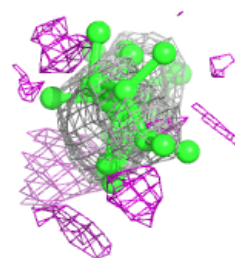
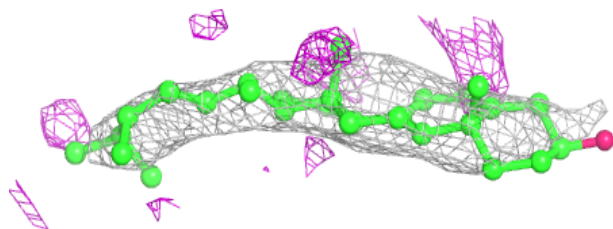
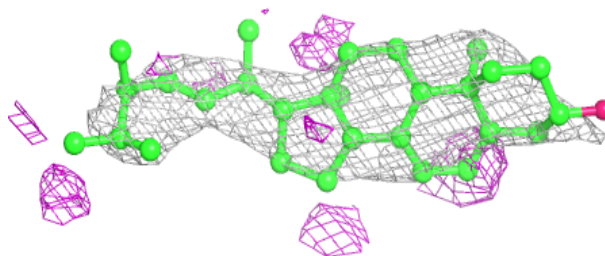


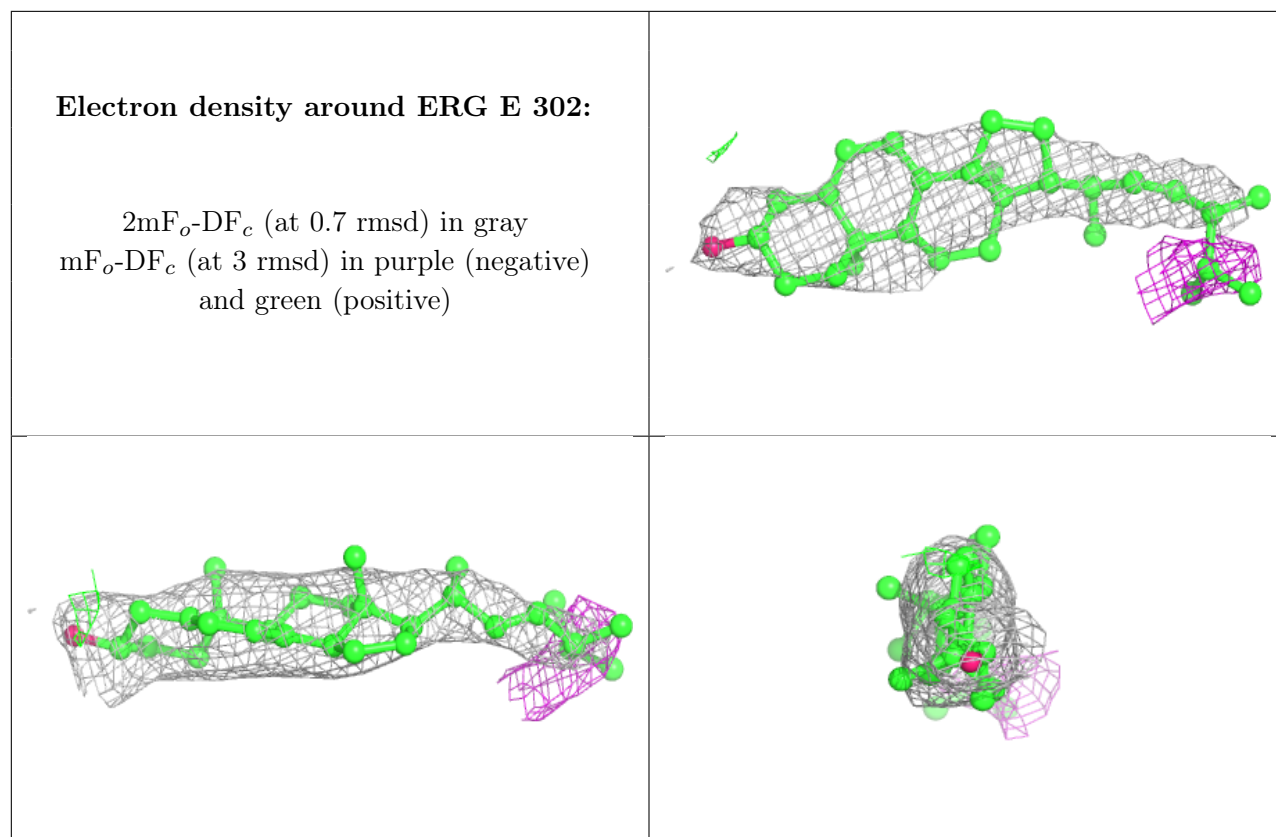
Electron density around ERG I 304:

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

**Electron density around ERG C 302:**

$2mF_o-DF_c$ (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.