Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 02:59 PM JST

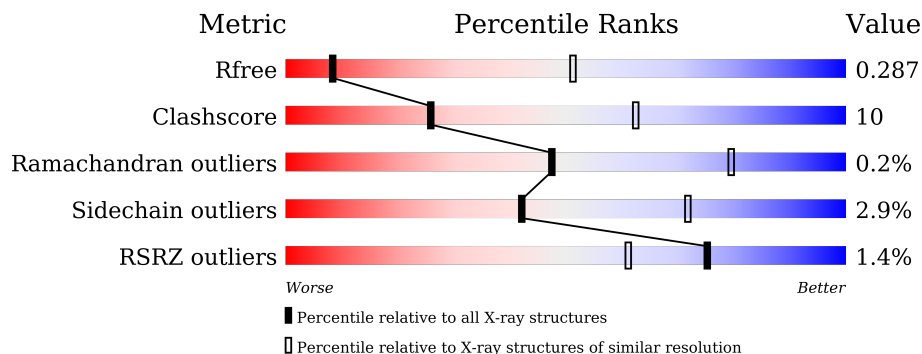|		
PDB ID	:	6L07
Title	:	Crystal structure of Escherichia coli phosphatidylserine decarboxylase (PE-bound form)
Authors	:	Watanabe, Y.; Watanabe, S.
Deposited on	:	2019-09-26
Resolution	:	3.60 Å(reported)

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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 3.60 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	Percentile Ranks	Value
Rfree		0.287
Clashscore		10
Ramachandran outliers		0.2%
Sidechain outliers		2.9%
RSRZ outliers		1.4%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	267	69% 26% • •
1	B	267	75% 20% •
1	C	267	70% 25% •
1	D	267	71% 24% • •
1	E	267	% 69% 26% • •
1	F	267	69% 26% • •

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Mol	Chain	Length	Quality of chain
1	G	267	% 64% 31% ••
1	H	267	6% 69% 26% •
2	I	36	67% 31% •
2	J	36	78% 19% •
2	K	36	69% 28% •
2	L	36	78% 19% •
2	M	36	64% 31% 6%
3	N	36	3% 61% 36% •
3	O	36	3% 61% 36% •
3	P	36	14% 75% 19% ••

2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 18179 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 Phosphatidylserine decarboxylase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2025	1308	346	361	10			
1	B	255	Total	C	N	O	S	0	0	0
			2022	1307	346	359	10			
1	C	255	Total	C	N	O	S	0	0	0
			2005	1297	345	353	10			
1	D	255	Total	C	N	O	S	0	0	0
			2018	1304	344	360	10			
1	E	255	Total	C	N	O	S	0	0	0
			2013	1303	344	356	10			
1	F	255	Total	C	N	O	S	0	0	0
			2014	1302	346	357	9			
1	G	255	Total	C	N	O	S	0	0	0
			2022	1305	346	361	10			
1	H	255	Total	C	N	O	S	0	0	0
			1998	1289	343	356	10			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A446DLT6
A	-12	GLY	-	expression tag	UNP A0A446DLT6
A	-11	SER	-	expression tag	UNP A0A446DLT6
A	-10	SER	-	expression tag	UNP A0A446DLT6
A	-9	HIS	-	expression tag	UNP A0A446DLT6
A	-8	HIS	-	expression tag	UNP A0A446DLT6
A	-7	HIS	-	expression tag	UNP A0A446DLT6
A	-6	HIS	-	expression tag	UNP A0A446DLT6
A	-5	HIS	-	expression tag	UNP A0A446DLT6
A	-4	HIS	-	expression tag	UNP A0A446DLT6
A	-3	SER	-	expression tag	UNP A0A446DLT6
A	-2	GLN	-	expression tag	UNP A0A446DLT6
A	-1	ASP	-	expression tag	UNP A0A446DLT6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	expression tag	UNP A0A446DLT6
B	-13	MET	-	expression tag	UNP A0A446DLT6
B	-12	GLY	-	expression tag	UNP A0A446DLT6
B	-11	SER	-	expression tag	UNP A0A446DLT6
B	-10	SER	-	expression tag	UNP A0A446DLT6
B	-9	HIS	-	expression tag	UNP A0A446DLT6
B	-8	HIS	-	expression tag	UNP A0A446DLT6
B	-7	HIS	-	expression tag	UNP A0A446DLT6
B	-6	HIS	-	expression tag	UNP A0A446DLT6
B	-5	HIS	-	expression tag	UNP A0A446DLT6
B	-4	HIS	-	expression tag	UNP A0A446DLT6
B	-3	SER	-	expression tag	UNP A0A446DLT6
B	-2	GLN	-	expression tag	UNP A0A446DLT6
B	-1	ASP	-	expression tag	UNP A0A446DLT6
B	0	PRO	-	expression tag	UNP A0A446DLT6
C	-13	MET	-	expression tag	UNP A0A446DLT6
C	-12	GLY	-	expression tag	UNP A0A446DLT6
C	-11	SER	-	expression tag	UNP A0A446DLT6
C	-10	SER	-	expression tag	UNP A0A446DLT6
C	-9	HIS	-	expression tag	UNP A0A446DLT6
C	-8	HIS	-	expression tag	UNP A0A446DLT6
C	-7	HIS	-	expression tag	UNP A0A446DLT6
C	-6	HIS	-	expression tag	UNP A0A446DLT6
C	-5	HIS	-	expression tag	UNP A0A446DLT6
C	-4	HIS	-	expression tag	UNP A0A446DLT6
C	-3	SER	-	expression tag	UNP A0A446DLT6
C	-2	GLN	-	expression tag	UNP A0A446DLT6
C	-1	ASP	-	expression tag	UNP A0A446DLT6
C	0	PRO	-	expression tag	UNP A0A446DLT6
D	-13	MET	-	expression tag	UNP A0A446DLT6
D	-12	GLY	-	expression tag	UNP A0A446DLT6
D	-11	SER	-	expression tag	UNP A0A446DLT6
D	-10	SER	-	expression tag	UNP A0A446DLT6
D	-9	HIS	-	expression tag	UNP A0A446DLT6
D	-8	HIS	-	expression tag	UNP A0A446DLT6
D	-7	HIS	-	expression tag	UNP A0A446DLT6
D	-6	HIS	-	expression tag	UNP A0A446DLT6
D	-5	HIS	-	expression tag	UNP A0A446DLT6
D	-4	HIS	-	expression tag	UNP A0A446DLT6
D	-3	SER	-	expression tag	UNP A0A446DLT6
D	-2	GLN	-	expression tag	UNP A0A446DLT6
D	-1	ASP	-	expression tag	UNP A0A446DLT6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PRO	-	expression tag	UNP A0A446DLT6
E	-13	MET	-	expression tag	UNP A0A446DLT6
E	-12	GLY	-	expression tag	UNP A0A446DLT6
E	-11	SER	-	expression tag	UNP A0A446DLT6
E	-10	SER	-	expression tag	UNP A0A446DLT6
E	-9	HIS	-	expression tag	UNP A0A446DLT6
E	-8	HIS	-	expression tag	UNP A0A446DLT6
E	-7	HIS	-	expression tag	UNP A0A446DLT6
E	-6	HIS	-	expression tag	UNP A0A446DLT6
E	-5	HIS	-	expression tag	UNP A0A446DLT6
E	-4	HIS	-	expression tag	UNP A0A446DLT6
E	-3	SER	-	expression tag	UNP A0A446DLT6
E	-2	GLN	-	expression tag	UNP A0A446DLT6
E	-1	ASP	-	expression tag	UNP A0A446DLT6
E	0	PRO	-	expression tag	UNP A0A446DLT6
F	-13	MET	-	expression tag	UNP A0A446DLT6
F	-12	GLY	-	expression tag	UNP A0A446DLT6
F	-11	SER	-	expression tag	UNP A0A446DLT6
F	-10	SER	-	expression tag	UNP A0A446DLT6
F	-9	HIS	-	expression tag	UNP A0A446DLT6
F	-8	HIS	-	expression tag	UNP A0A446DLT6
F	-7	HIS	-	expression tag	UNP A0A446DLT6
F	-6	HIS	-	expression tag	UNP A0A446DLT6
F	-5	HIS	-	expression tag	UNP A0A446DLT6
F	-4	HIS	-	expression tag	UNP A0A446DLT6
F	-3	SER	-	expression tag	UNP A0A446DLT6
F	-2	GLN	-	expression tag	UNP A0A446DLT6
F	-1	ASP	-	expression tag	UNP A0A446DLT6
F	0	PRO	-	expression tag	UNP A0A446DLT6
G	-13	MET	-	expression tag	UNP A0A446DLT6
G	-12	GLY	-	expression tag	UNP A0A446DLT6
G	-11	SER	-	expression tag	UNP A0A446DLT6
G	-10	SER	-	expression tag	UNP A0A446DLT6
G	-9	HIS	-	expression tag	UNP A0A446DLT6
G	-8	HIS	-	expression tag	UNP A0A446DLT6
G	-7	HIS	-	expression tag	UNP A0A446DLT6
G	-6	HIS	-	expression tag	UNP A0A446DLT6
G	-5	HIS	-	expression tag	UNP A0A446DLT6
G	-4	HIS	-	expression tag	UNP A0A446DLT6
G	-3	SER	-	expression tag	UNP A0A446DLT6
G	-2	GLN	-	expression tag	UNP A0A446DLT6
G	-1	ASP	-	expression tag	UNP A0A446DLT6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	PRO	-	expression tag	UNP A0A446DLT6
H	-13	MET	-	expression tag	UNP A0A446DLT6
H	-12	GLY	-	expression tag	UNP A0A446DLT6
H	-11	SER	-	expression tag	UNP A0A446DLT6
H	-10	SER	-	expression tag	UNP A0A446DLT6
H	-9	HIS	-	expression tag	UNP A0A446DLT6
H	-8	HIS	-	expression tag	UNP A0A446DLT6
H	-7	HIS	-	expression tag	UNP A0A446DLT6
H	-6	HIS	-	expression tag	UNP A0A446DLT6
H	-5	HIS	-	expression tag	UNP A0A446DLT6
H	-4	HIS	-	expression tag	UNP A0A446DLT6
H	-3	SER	-	expression tag	UNP A0A446DLT6
H	-2	GLN	-	expression tag	UNP A0A446DLT6
H	-1	ASP	-	expression tag	UNP A0A446DLT6
H	0	PRO	-	expression tag	UNP A0A446DLT6

- Molecule 2 is a protein called Phosphatidylserine decarboxylase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	35	Total 244	C 159	N 39	O 46	0	0	0
2	J	35	Total 244	C 159	N 39	O 46	0	0	0
2	K	35	Total 244	C 159	N 39	O 46	0	0	0
2	L	35	Total 244	C 159	N 39	O 46	0	0	0
2	M	34	Total 239	C 156	N 38	O 45	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	254	PPI	SER	modified residue	UNP A0A446DLT6
J	254	PPI	SER	modified residue	UNP A0A446DLT6
K	254	PPI	SER	modified residue	UNP A0A446DLT6
L	254	PPI	SER	modified residue	UNP A0A446DLT6
M	254	PPI	SER	modified residue	UNP A0A446DLT6

- Molecule 3 is a protein called Phosphatidylserine decarboxylase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	N	35	Total	C	N	O	0	0	0
			245	159	39	47			
3	O	35	Total	C	N	O	0	0	0
			245	159	39	47			
3	P	35	Total	C	N	O	0	0	0
			242	156	39	47			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	254	PYR	SER	modified residue	UNP A0A446DLT6
O	254	PYR	SER	modified residue	UNP A0A446DLT6
P	254	PYR	SER	modified residue	UNP A0A446DLT6

- Molecule 4 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).

PEE

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	I	1	Total	C	N	O	P	0	0
			23	13	1	8	1		
4	J	1	Total	C	N	O	P	0	0
			23	13	1	8	1		
4	K	1	Total	C	N	O	P	0	0
			23	13	1	8	1		
4	L	1	Total	C	N	O	P	0	0
			23	13	1	8	1		
4	M	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

3 Residue-property plots ⓘ

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.
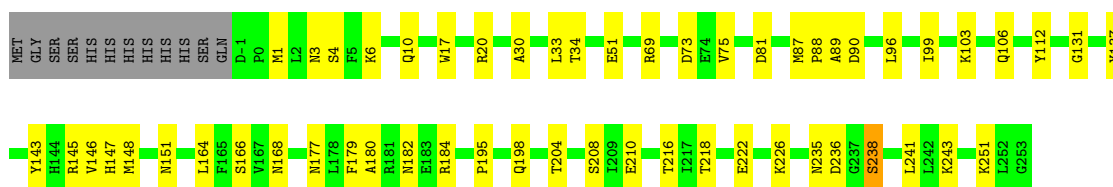
• Molecule 1: Phosphatidylserine decarboxylase beta chain
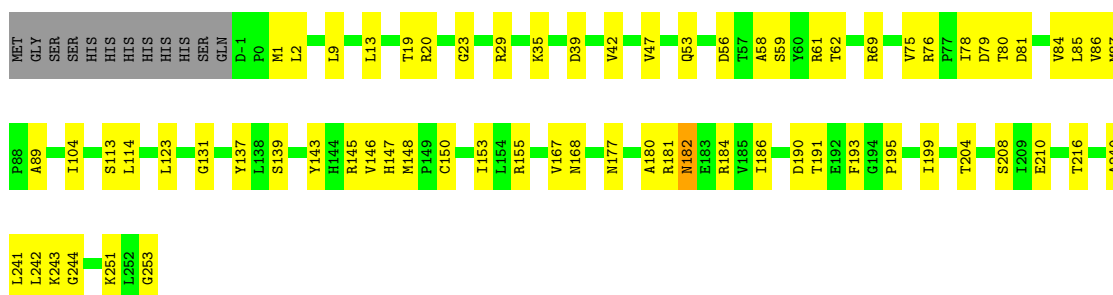
Chain A:

• Molecule 1: Phosphatidylserine decarboxylase beta chain

Chain B:

• Molecule 1: Phosphatidylserine decarboxylase beta chain

Chain C:

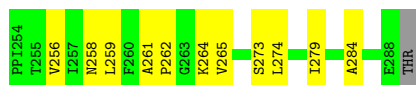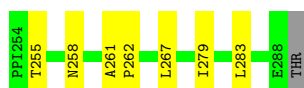
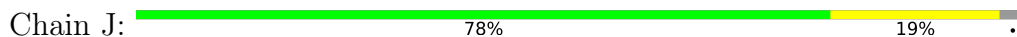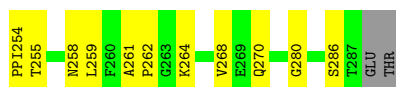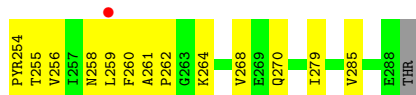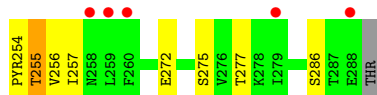• Molecule 1: Phosphatidylserine decarboxylase beta chain

Chain D:　　　　71%　　　　24%

MET GLY SER SER HIS HIS HIS HIS HIS SER GLN D-1 P0 M1 L2 N3 L7 S8 L9 Q10 Y11 I12 L13 P14 W17 R20 G23 A30 G31 W32 L33 T34 V37 I38 Q53 N64 E65 F66 R69 P70 L71 R72 V75 D81 V84 L85 V86

M87 D90 E101 D102 Q106 Y112 S113 L114 N130 G131 T135 T136 Y137 Y143 M148 P149 I153 L154 R155 Y159 V167 N168 Q173 D190 T191 E192 F193 A197 Q198 I205 E210 T211 T216 I217 K226 R227 G233 E234 N235 D236

A240 L241 M247 L252 G253

• Molecule 1: Phosphatidylserine decarboxylase beta chain

%

Chain E:　　　　69%　　　　26%

MET GLY SER SER HIS HIS HIS HIS HIS SER GLN D-1 F5 L9 Q10 Y11 I12 L13 P14 W17 L18 T19 R20 G23 L33 T34 K35 I38 V47 A52 A58 F66 R69 P70 L71 R72 V75 L85 V86 M87 P88 A89 I99 I104

L105 Q106 Y112 S113 L114 Y122 F128 R129 N130 G131 Y137 L138 R141 D142 Y143 H144 R145 V146 M147 M148 P149 C150 N151 G152 I153 E156 M157 L164 F165 S166 V167 N168 H169 L170 T171 N174 L178 N182 C187 A197 G202 A203 T204 I205 S208 I209

E210 T216 R221 E222 G223 T229 G233 E234 N235 D236 A240 L241 L242 K243 K251 L252 G253

• Molecule 1: Phosphatidylserine decarboxylase beta chain

Chain F:　　　　69%　　　　26%

MET GLY SER SER HIS HIS HIS HIS HIS SER GLN D-1 P0 M1 L2 N3 S4 F5 K6 L7 S8 L13 P14 K15 L16 W17 R20 K35 I38 D39 Y45 A52 N64 E65 F66 F67 V68 L71 R72 D73 E74 V75 R76 V84 L85 V86 M87 P88 A89 D90

I99 K103 Q106 Y112 S113 L114 F128 G131 V134 T135 T136 Y137 R141 D142 Y143 H144 R145 V146 M147 M148 I153 I158 P161 V167 L170 N174 F179 A180 R181 N182 I186 P195 M196 A197 I205 S208 I209 E210 G223 I224

I225 G233 E234 S238 V239 A240 L241 L242 K243 E246 R249 F250 K251 L252 G253

• Molecule 1: Phosphatidylserine decarboxylase beta chain

%

Chain G:　　　　64%　　　　31%

MET GLY SER SER HIS HIS HIS HIS HIS SER GLN D-1 L2 N3 S4 F5 K6 L7 S8 L9 Q10 L13 P14 K15 T19 R20 R29 A30 G31 W32 L33 T34 K35 L36 V37 I38 V42 V47 A58 S59 Y60 R61 T62 E65 R69 D73 E74 V75 R76

P77 D81 V84 P88 G91 K98 I99 I104 L105 Q106 Y112 S113 L114 L117 Y122 L123 M124 A125 F128 R129 N130 G131 T132 D142 Y143 H144 R145 N151 R155 Y159 S166 V167 N168 N177 L178 F179 A180 E183 I186 D190 T191

E192 F193 A197 Q198 I199 T204 I205 V206 G207 S208 I209 P219 P220 R221 E222 G223 K226 A232 D236 E246 R249 F250 K251 L252 G253

• Molecule 1: Phosphatidylserine decarboxylase beta chain

Chain H:

6%
69%   26%

MET GLY SER HIS HIS HIS HIS HIS SER GLN D-1 P0 M1 L9 Q10 L13 P14 K15 R20 R29 T34 K35 I38 D39 L40 V47 T57 R61 T62 F63 F66 R69 P70 L71 V75 R76 D81 V84 L85 V86 M87 I93 S94

Q95 L96 G97 K98 I104 L105 Q106 Y112 S113 L114 A119 D126 R129 T132 T135 T136 Y137 R141 D142 Y143 H144 R145 V146 M147 M148 P149 C150 N151 L154 R155 P161 S166 V167 N168 H169 L170 N177 L178 F179 A180 R181 C187 L188 F189 D190 T191 E192

F193 G194 P195 M196 A197 Q198 I199 I205 V206 E210 T211 T216 I217 G223 I224 I225 L241 L242 K243 G248 R249 F250 G253

• Molecule 2: Phosphatidylserine decarboxylase alpha chain

Chain I:

67%   31%

PPI254 T255 V256 I257 N258 L259 F260 A261 P262 G263 K264 V265 S273 L274 I279 A284 E288 THR

• Molecule 2: Phosphatidylserine decarboxylase alpha chain

Chain J:

78%   19%

PPI254 T255 N258 A261 P262 L267 I279 L283 E288 THR

• Molecule 2: Phosphatidylserine decarboxylase alpha chain

Chain K:

69%   28%

PPI254 T255 V256 I257 A261 P262 V265 V268 L271 P282 L283 A284 E288 THR

• Molecule 2: Phosphatidylserine decarboxylase alpha chain

Chain L:

78%   19%

PPI254 L259 F260 A261 P262 G263 K264 T277 K278 I279 G280 Q281 E288 THR

• Molecule 2: Phosphatidylserine decarboxylase alpha chain

Chain M:

64%	31%	6%

PPI254 T255 N258 L259 F260 A261 P262 G263 K264 V268 E269 Q270 G280 S286 T287 GLU THR

• Molecule 3: Phosphatidylserine decarboxylase alpha chain

3%

Chain N:

61%	36%

PYR254 N258 L259 P262 V265 N266 L267 S273 L274 T277 K278 I279 G280 Q281 P282 L283 A284 V285 S286 T287 E288 THR

• Molecule 3: Phosphatidylserine decarboxylase alpha chain

3%

Chain O:

61%	36%

PYR254 T255 V256 I257 N258 L259 F260 A261 P262 G263 K264 V268 E269 Q270 I279 V285 E288 THR

• Molecule 3: Phosphatidylserine decarboxylase alpha chain

14%

Chain P:

75%	19%

PYR254 T255 V256 I257 N258 L259 F260 E272 S275 V276 T277 K278 I279 S286 T287 E288 THR

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	218.19Å 218.19Å 143.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.24 – 3.60 49.24 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.24-3.60) 99.9 (49.24-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.241 , 0.289 0.239 , 0.287	Depositor DCC
R_{free} test set	2328 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	160.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 98.5	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18179	wwPDB-VP
Average B, all atoms (Å^2)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PPI, PYR, PEE

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	0.27	0/2076	0.49	0/2819
1	B	0.25	0/2073	0.45	0/2815
1	C	0.25	0/2056	0.44	0/2795
1	D	0.24	0/2069	0.46	0/2811
1	E	0.25	0/2064	0.47	0/2805
1	F	0.24	0/2065	0.47	0/2806
1	G	0.25	0/2073	0.46	0/2815
1	H	0.24	0/2048	0.45	0/2785
2	I	0.24	0/242	0.50	0/331
2	J	0.24	0/242	0.49	0/331
2	K	0.25	0/242	0.46	0/331
2	L	0.24	0/242	0.50	0/331
2	M	0.26	0/237	0.51	0/324
3	N	0.24	0/242	0.49	0/331
3	O	0.23	0/242	0.45	0/331
3	P	0.23	0/239	0.46	0/327
All	All	0.25	0/18452	0.46	0/25088

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
3	O	0	1
3	P	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	O	254	PYR	Peptide
3	P	254	PYR	Peptide

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	2025	0	2036	54	0
1	B	2022	0	2034	32	0
1	C	2005	0	2000	44	0
1	D	2018	0	2021	43	0
1	E	2013	0	2013	50	0
1	F	2014	0	2021	47	0
1	G	2022	0	2027	59	0
1	H	1998	0	1988	47	0
2	I	244	0	258	9	0
2	J	244	0	258	10	0
2	K	244	0	258	9	0
2	L	244	0	258	6	0
2	M	239	0	256	11	0
3	N	245	0	255	11	0
3	O	245	0	255	15	0
3	P	242	0	246	9	0
4	I	23	0	18	7	0
4	J	23	0	19	1	0
4	K	23	0	18	3	0
4	L	23	0	18	5	0
4	M	23	0	18	3	0
All	All	18179	0	18275	382	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 10.

All (382) 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:99:ILE:HD13	1:A:104:ILE:HG12	1.54	0.88
1:A:131:GLY:HA2	2:I:262:PRO:HA	1.54	0.86
1:A:205:ILE:HD11	4:I:301:PEE:H49	1.62	0.80
1:A:30:ALA:HB3	1:A:34:THR:HG23	1.66	0.77
1:H:135:THR:HA	3:P:257:ILE:HG22	1.65	0.76
1:D:210:GLU:HB3	1:D:216:THR:HA	1.67	0.75
1:C:181:ARG:HD3	1:G:223:GLY:HA3	1.69	0.74
1:E:168:ASN:HD21	1:E:170:LEU:HB2	1.53	0.73
1:E:10:GLN:NE2	1:E:166:SER:OG	2.21	0.73
1:A:41:PHE:HD2	1:A:63:PHE:HZ	1.34	0.72
1:C:195:PRO:HD2	2:K:261:ALA:HB2	1.71	0.72
1:A:19:THR:HG23	1:A:205:ILE:HA	1.70	0.72
1:A:30:ALA:HB1	1:A:33:LEU:HB3	1.73	0.71
1:A:195:PRO:HD2	2:I:261:ALA:HB2	1.73	0.71
1:E:210:GLU:HB3	1:E:216:THR:HA	1.73	0.70
1:A:208:SER:HB3	1:A:251:LYS:HB3	1.72	0.70
1:E:89:ALA:HA	2:L:279:ILE:HG12	1.71	0.70
1:F:234:GLU:HG2	1:G:61:ARG:HH12	1.55	0.69
1:G:155:ARG:NH1	1:G:190:ASP:OD2	2.25	0.69
1:E:131:GLY:HA2	2:L:262:PRO:HA	1.74	0.69
1:E:19:THR:HG21	1:E:164:LEU:HD13	1.74	0.69
1:E:170:LEU:O	1:E:174:ASN:ND2	2.24	0.69
1:H:29:ARG:HH21	1:H:61:ARG:HD3	1.56	0.68
1:F:181:ARG:HD3	1:H:223:GLY:HA3	1.74	0.68
1:G:35:LYS:HE2	1:G:58:ALA:HB2	1.73	0.68
1:C:29:ARG:HH21	1:C:61:ARG:HD3	1.59	0.68
1:G:205:ILE:HG22	1:G:252:LEU:HG	1.75	0.68
1:H:98:LYS:HA	1:H:132:THR:HA	1.77	0.67
1:E:165:PHE:H	1:E:182:ASN:HD21	1.43	0.67
1:F:131:GLY:HA2	3:O:262:PRO:HA	1.78	0.66
1:C:186:ILE:HG23	1:C:199:ILE:HG12	1.76	0.66
1:E:166:SER:HB2	1:E:171:THR:HG21	1.78	0.66
1:D:233:GLY:O	1:D:235:ASN:ND2	2.29	0.66
1:G:10:GLN:NE2	1:G:166:SER:OG	2.27	0.66
1:H:126:ASP:HA	1:H:129:ARG:HD3	1.77	0.66
1:D:155:ARG:NH1	1:D:190:ASP:OD2	2.27	0.65
1:G:191:THR:HG23	1:G:193:PHE:H	1.61	0.65
1:D:14:PRO:HB2	1:D:17:TRP:HB2	1.79	0.65
1:C:199:ILE:HB	2:K:257:ILE:HG22	1.78	0.64
1:C:35:LYS:HE2	1:C:58:ALA:HB2	1.78	0.64
1:F:197:ALA:HB3	3:O:259:LEU:HB2	1.78	0.64
1:G:197:ALA:HB3	2:M:259:LEU:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:GLY:HA2	2:J:262:PRO:HA	1.80	0.64
1:C:210:GLU:HB3	1:C:216:THR:HA	1.80	0.64
4:I:301:PEE:O1P	4:I:301:PEE:H7	1.98	0.64
1:C:1:MET:HG3	1:C:2:LEU:HD12	1.80	0.63
1:B:30:ALA:HB3	1:B:34:THR:HG23	1.81	0.63
1:D:86:VAL:HG22	3:N:279:ILE:O	1.98	0.63
1:C:155:ARG:NH1	1:C:190:ASP:OD2	2.27	0.62
1:A:181:ARG:HD3	1:E:223:GLY:HA3	1.81	0.62
1:A:101:GLU:OE2	1:D:227:ARG:NH1	2.32	0.62
1:G:42:VAL:HG13	1:G:47:VAL:HB	1.79	0.62
1:G:30:ALA:O	1:G:34:THR:OG1	2.16	0.62
1:D:137:TYR:HE1	1:D:167:VAL:HG13	1.64	0.62
1:D:191:THR:HG23	1:D:193:PHE:H	1.65	0.61
1:C:123:LEU:HD11	1:G:123:LEU:HD11	1.82	0.61
1:C:131:GLY:HA2	2:K:262:PRO:HA	1.82	0.61
1:G:29:ARG:HH21	1:G:61:ARG:HH11	1.49	0.61
1:C:177:ASN:HB3	1:C:180:ALA:HB3	1.83	0.60
1:E:23:GLY:HA3	1:E:253:GLY:HA2	1.83	0.60
1:E:197:ALA:HB3	2:L:259:LEU:HB2	1.82	0.60
1:H:155:ARG:NH1	1:H:190:ASP:OD2	2.35	0.60
1:F:223:GLY:HA3	1:H:181:ARG:HD3	1.82	0.60
1:C:89:ALA:HB2	1:C:146:VAL:HG13	1.83	0.60
1:D:87:MET:HA	3:N:283:LEU:HD22	1.83	0.60
1:A:14:PRO:HB2	1:A:17:TRP:HD1	1.66	0.60
1:D:30:ALA:HB3	1:D:34:THR:HG23	1.84	0.60
4:I:301:PEE:H7	4:I:301:PEE:P	2.41	0.59
1:B:198:GLN:OE1	2:J:258:ASN:ND2	2.35	0.59
1:G:9:LEU:HG	1:G:13:LEU:HD23	1.84	0.59
1:C:147:HIS:ND1	1:C:244:GLY:O	2.34	0.59
1:D:131:GLY:HA2	3:N:262:PRO:HA	1.83	0.59
1:C:19:THR:OG1	1:C:204:THR:O	2.19	0.59
1:C:182:ASN:O	1:C:184:ARG:NH1	2.36	0.58
1:C:204:THR:HG22	4:K:301:PEE:H1	1.84	0.58
1:F:90:ASP:OD1	3:O:279:ILE:HG13	2.04	0.58
1:C:208:SER:HB3	1:C:251:LYS:HB3	1.85	0.58
1:A:1:MET:HA	1:A:4:SER:HB3	1.86	0.58
2:M:261:ALA:HB3	2:M:264:LYS:HG2	1.85	0.58
1:C:204:THR:HG21	4:K:301:PEE:H49	1.86	0.58
1:E:35:LYS:HE2	1:E:58:ALA:HB2	1.86	0.58
1:A:205:ILE:CD1	4:I:301:PEE:H49	2.33	0.58
1:G:98:LYS:HA	1:G:132:THR:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASP:O	1:A:59:SER:OG	2.20	0.58
1:F:153:ILE:HG13	1:F:240:ALA:HB2	1.86	0.57
1:H:71:LEU:HD22	1:H:75:VAL:HG11	1.86	0.57
1:G:222:GLU:OE1	1:G:226:LYS:NZ	2.28	0.57
1:E:14:PRO:HB2	1:E:17:TRP:HD1	1.69	0.57
1:D:9:LEU:O	1:D:13:LEU:HG	2.05	0.57
1:H:191:THR:HG23	1:H:193:PHE:H	1.70	0.56
1:G:81:ASP:HB3	1:G:84:VAL:HG22	1.86	0.56
1:G:177:ASN:HB3	1:G:180:ALA:HB3	1.85	0.56
1:C:56:ASP:O	1:C:59:SER:OG	2.23	0.56
1:A:3:ASN:O	1:A:6:LYS:N	2.37	0.56
1:F:137:TYR:HE1	1:F:167:VAL:HG13	1.70	0.56
1:C:35:LYS:NZ	1:C:39:ASP:OD2	2.34	0.56
1:D:205:ILE:HG22	1:D:252:LEU:HG	1.88	0.56
1:F:89:ALA:HA	3:O:279:ILE:HG12	1.88	0.56
1:D:87:MET:HG2	3:N:281:GLN:O	2.06	0.55
1:G:208:SER:HB3	1:G:251:LYS:HB3	1.88	0.55
1:A:30:ALA:O	1:A:34:THR:OG1	2.19	0.55
1:E:10:GLN:OE1	1:E:166:SER:N	2.34	0.55
1:G:30:ALA:HB3	1:G:34:THR:HG23	1.87	0.55
1:B:182:ASN:O	1:B:184:ARG:NH1	2.40	0.55
1:C:104:ILE:HD11	1:C:114:LEU:HD13	1.88	0.55
1:C:191:THR:HG23	1:C:193:PHE:H	1.73	0.54
1:G:104:ILE:HD11	1:G:114:LEU:HD13	1.89	0.54
1:F:99:ILE:HG13	1:F:103:LYS:O	2.08	0.54
1:H:75:VAL:HG13	1:H:76:ARG:HG2	1.88	0.54
1:A:23:GLY:HA3	1:A:253:GLY:HA2	1.89	0.54
1:G:13:LEU:O	1:G:15:LYS:NZ	2.38	0.54
1:H:87:MET:SD	3:P:277:THR:HG23	2.48	0.54
1:E:156:GLU:HG2	1:E:229:THR:HG22	1.90	0.54
1:B:10:GLN:NE2	1:B:166:SER:OG	2.40	0.54
1:B:90:ASP:OD1	2:J:279:ILE:HG13	2.08	0.54
1:E:14:PRO:HB2	1:E:17:TRP:CD1	2.43	0.54
1:F:85:LEU:HD22	3:O:260:PHE:HE2	1.73	0.54
1:C:23:GLY:HA3	1:C:253:GLY:HA2	1.90	0.54
1:E:47:VAL:HG22	1:E:141:ARG:HA	1.89	0.53
1:G:29:ARG:NH2	1:G:61:ARG:HD3	2.23	0.53
1:G:32:TRP:O	1:G:36:LEU:N	2.35	0.53
2:K:265:VAL:HG13	2:K:284:ALA:HB1	1.91	0.53
1:F:208:SER:HB3	1:F:251:LYS:HB3	1.91	0.53
1:E:204:THR:HG21	4:L:301:PEE:H14	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASP:OD1	1:A:80:THR:N	2.41	0.53
1:F:75:VAL:HG13	1:F:76:ARG:HG2	1.90	0.53
1:G:99:ILE:N	1:G:131:GLY:O	2.40	0.53
1:C:85:LEU:O	2:K:283:LEU:N	2.39	0.53
2:I:265:VAL:HG13	2:I:284:ALA:HB1	1.91	0.53
1:G:145:ARG:NH1	1:G:246:GLU:OE2	2.34	0.53
1:D:81:ASP:HB3	1:D:84:VAL:HG22	1.91	0.53
1:A:3:ASN:O	1:A:7:LEU:HD23	2.09	0.53
1:A:114:LEU:HD21	1:A:128:PHE:HB2	1.91	0.53
1:B:222:GLU:OE1	1:B:226:LYS:NZ	2.33	0.53
1:G:4:SER:HA	1:G:7:LEU:HB2	1.90	0.53
2:M:268:VAL:HG12	2:M:270:GLN:H	1.72	0.52
1:A:148:MET:HG3	1:A:241:LEU:HG	1.92	0.52
1:D:153:ILE:HG13	1:D:240:ALA:HB2	1.89	0.52
1:A:74:GLU:HA	1:C:242:LEU:HD13	1.91	0.52
1:F:134:VAL:HG13	3:O:258:ASN:HB2	1.90	0.52
1:F:148:MET:HG3	1:F:241:LEU:HG	1.90	0.52
1:A:204:THR:HG21	4:I:301:PEE:H14	1.92	0.52
1:H:47:VAL:HA	1:H:141:ARG:HG3	1.91	0.52
1:B:208:SER:HB3	1:B:251:LYS:HB3	1.92	0.52
1:E:114:LEU:HD21	1:E:128:PHE:HB2	1.92	0.51
1:E:168:ASN:ND2	1:E:170:LEU:HB2	2.24	0.51
1:H:148:MET:HE3	1:H:149:PRO:HD2	1.92	0.51
1:C:148:MET:HG3	1:C:241:LEU:HG	1.93	0.51
1:B:88:PRO:HD3	2:J:283:LEU:HD22	1.93	0.51
1:E:38:ILE:HG12	1:E:66:PHE:CD2	2.45	0.51
1:F:114:LEU:HD21	1:F:128:PHE:HB2	1.92	0.51
1:E:208:SER:HB3	1:E:251:LYS:HB3	1.93	0.51
1:H:-1:ASP:OD1	1:H:-1:ASP:N	2.38	0.51
1:H:9:LEU:O	1:H:13:LEU:HB2	2.11	0.51
1:G:112:TYR:HE2	1:G:117:LEU:HD22	1.76	0.51
1:G:151:ASN:O	1:G:191:THR:OG1	2.21	0.51
1:C:153:ILE:HG13	1:C:240:ALA:HB2	1.92	0.51
1:H:13:LEU:HD12	1:H:14:PRO:HD2	1.93	0.51
1:B:210:GLU:HB3	1:B:216:THR:HA	1.93	0.50
1:A:85:LEU:N	2:I:284:ALA:O	2.27	0.50
1:A:165:PHE:HB2	1:A:178:LEU:HD11	1.93	0.50
1:F:143:TYR:CZ	1:F:145:ARG:HB2	2.46	0.50
1:H:143:TYR:CZ	1:H:145:ARG:HB2	2.45	0.50
1:D:23:GLY:HA3	1:D:253:GLY:HA2	1.92	0.50
1:D:148:MET:HG3	1:D:241:LEU:HG	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:PRO:HB2	1:A:17:TRP:CD1	2.46	0.50
1:G:114:LEU:HD21	1:G:128:PHE:HB2	1.94	0.50
1:A:136:THR:HB	2:I:256:VAL:HG12	1.93	0.50
1:G:168:ASN:N	4:M:301:PEE:O2P	2.44	0.50
1:A:78:ILE:HG12	1:A:244:GLY:HA3	1.94	0.50
1:D:102:ASP:OD1	1:D:114:LEU:N	2.43	0.50
1:H:179:PHE:HE1	3:P:255:THR:HG21	1.76	0.50
1:D:101:GLU:HG2	1:D:130:ASN:OD1	2.12	0.50
1:F:136:THR:HB	3:O:256:VAL:HG22	1.94	0.49
1:A:41:PHE:CD2	1:A:63:PHE:HZ	2.22	0.49
1:E:137:TYR:OH	4:L:301:PEE:O2P	2.24	0.49
1:F:35:LYS:NZ	1:F:39:ASP:OD2	2.45	0.49
1:E:87:MET:HG3	2:L:281:GLN:HB2	1.95	0.49
1:G:29:ARG:HA	1:G:62:THR:HG22	1.94	0.49
1:G:106:GLN:HB2	1:G:112:TYR:CE1	2.47	0.49
1:A:203:ALA:HB3	1:A:206:VAL:HB	1.93	0.49
1:E:9:LEU:HA	1:E:12:ILE:HG22	1.93	0.49
1:H:161:PRO:HD2	1:H:225:ILE:HG12	1.94	0.49
2:L:261:ALA:HB3	2:L:264:LYS:HB2	1.95	0.49
1:F:15:LYS:H	1:F:15:LYS:HD3	1.78	0.49
1:F:3:ASN:HB3	1:F:170:LEU:HD11	1.93	0.49
1:F:161:PRO:HD2	1:F:225:ILE:HG12	1.94	0.49
1:D:191:THR:HG23	1:D:193:PHE:N	2.28	0.48
1:F:145:ARG:NH1	1:F:246:GLU:OE2	2.40	0.48
1:A:11:TYR:CE1	1:E:17:TRP:HH2	2.30	0.48
1:D:101:GLU:O	1:D:102:ASP:HB3	2.13	0.48
1:E:153:ILE:HG13	1:E:240:ALA:HB2	1.96	0.48
1:F:144:HIS:O	1:F:249:ARG:HB2	2.13	0.48
1:F:147:HIS:CD2	3:O:279:ILE:HD13	2.47	0.48
1:F:170:LEU:O	1:F:174:ASN:ND2	2.46	0.48
1:H:10:GLN:OE1	1:H:166:SER:N	2.36	0.48
1:H:151:ASN:OD1	1:H:243:LYS:N	2.47	0.48
1:B:177:ASN:HB3	1:B:180:ALA:HB3	1.95	0.48
3:O:268:VAL:HG12	3:O:270:GLN:H	1.78	0.48
1:D:137:TYR:CE1	1:D:167:VAL:HG13	2.47	0.48
1:E:87:MET:SD	2:L:277:THR:HG23	2.53	0.48
1:G:2:LEU:O	1:G:5:PHE:HB2	2.13	0.48
1:A:99:ILE:HG23	1:A:131:GLY:H	1.78	0.48
1:G:179:PHE:CE1	2:M:255:THR:HG21	2.49	0.48
1:H:193:PHE:HE2	3:P:286:SER:HB2	1.79	0.48
1:F:158:ILE:HB	1:F:186:ILE:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ASP:HA	3:N:277:THR:O	2.13	0.48
1:E:104:ILE:HD11	1:E:114:LEU:HD13	1.95	0.48
1:F:73:ASP:OD1	1:F:74:GLU:N	2.46	0.48
1:G:29:ARG:HH21	1:G:61:ARG:HD3	1.77	0.47
1:G:143:TYR:CZ	1:G:145:ARG:HB2	2.49	0.47
1:D:198:GLN:OE1	3:N:258:ASN:ND2	2.41	0.47
1:E:99:ILE:O	1:E:130:ASN:HA	2.13	0.47
1:A:167:VAL:HG12	4:I:301:PEE:O4P	2.14	0.47
1:H:35:LYS:NZ	1:H:39:ASP:OD2	2.46	0.47
1:G:19:THR:OG1	1:G:204:THR:O	2.26	0.47
1:A:203:ALA:HB2	4:I:301:PEE:H12	1.97	0.47
3:O:264:LYS:HD2	3:O:264:LYS:HA	1.65	0.47
1:B:131:GLY:HA2	2:J:262:PRO:CA	2.44	0.47
1:F:179:PHE:CE1	3:O:255:THR:HG21	2.49	0.47
1:H:193:PHE:CE2	3:P:286:SER:HB2	2.50	0.47
1:G:130:ASN:O	2:M:262:PRO:HB3	2.15	0.47
1:C:9:LEU:HD11	1:C:13:LEU:HD13	1.96	0.46
1:E:9:LEU:HD23	1:E:10:GLN:H	1.80	0.46
1:E:143:TYR:CZ	1:E:145:ARG:HB2	2.51	0.46
1:H:114:LEU:HD23	1:H:129:ARG:HG3	1.96	0.46
1:D:72:ARG:O	1:D:75:VAL:HG12	2.15	0.46
1:E:138:LEU:O	4:L:301:PEE:H11	2.15	0.46
1:F:210:GLU:HG2	1:F:249:ARG:HG2	1.98	0.46
1:A:153:ILE:HG13	1:A:240:ALA:HB2	1.97	0.46
1:B:99:ILE:HG13	1:B:103:LYS:O	2.15	0.46
1:C:81:ASP:HB3	1:C:84:VAL:HG22	1.97	0.46
1:E:99:ILE:HG23	1:E:104:ILE:HG12	1.98	0.46
1:E:151:ASN:OD1	1:E:243:LYS:N	2.49	0.46
1:B:3:ASN:HA	1:B:6:LYS:HD3	1.97	0.46
1:C:168:ASN:N	4:K:301:PEE:O2P	2.49	0.46
1:G:60:TYR:HD1	1:G:65:GLU:HG2	1.81	0.46
1:C:143:TYR:CZ	1:C:145:ARG:HB2	2.50	0.45
3:O:258:ASN:HB3	3:O:260:PHE:CE1	2.50	0.45
1:G:38:ILE:O	1:G:42:VAL:HG23	2.16	0.45
1:G:131:GLY:HA2	2:M:262:PRO:HA	1.97	0.45
1:H:106:GLN:HB2	1:H:112:TYR:CD1	2.51	0.45
1:B:151:ASN:OD1	1:B:243:LYS:N	2.39	0.45
1:C:86:VAL:HA	2:K:282:PRO:HA	1.99	0.45
1:F:137:TYR:CE1	1:F:167:VAL:HG13	2.51	0.45
1:A:145:ARG:HG2	1:A:249:ARG:HB3	1.99	0.45
1:A:197:ALA:HB3	2:I:259:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ASP:OD1	1:C:80:THR:N	2.49	0.45
1:E:85:LEU:HD23	1:E:149:PRO:HB2	1.99	0.45
1:F:45:TYR:HB3	1:F:141:ARG:HB2	1.98	0.45
1:G:166:SER:OG	4:M:301:PEE:H13	2.16	0.45
1:D:193:PHE:HB3	3:N:265:VAL:HG23	1.98	0.45
1:F:4:SER:O	1:F:8:SER:N	2.38	0.45
1:H:95:GLN:H	1:H:135:THR:HB	1.80	0.45
1:F:225:ILE:HD12	1:H:119:ALA:HB1	1.98	0.45
1:H:81:ASP:HB3	1:H:84:VAL:HG22	1.97	0.45
1:D:106:GLN:HB2	1:D:112:TYR:CD1	2.51	0.45
1:B:137:TYR:OH	4:J:301:PEE:O1P	2.17	0.45
1:D:53:GLN:HB3	1:D:70:PRO:HG2	1.99	0.45
1:D:211:THR:HG23	1:D:217:ILE:HD11	2.00	0.44
1:F:14:PRO:HB2	1:F:17:TRP:HB2	1.99	0.44
1:C:78:ILE:HD12	1:C:78:ILE:H	1.82	0.44
1:D:90:ASP:OD2	1:D:143:TYR:HB3	2.18	0.44
1:F:52:ALA:HA	1:F:71:LEU:HD23	1.98	0.44
1:F:64:ASN:O	1:F:68:VAL:HG22	2.17	0.44
1:E:89:ALA:HB2	1:E:146:VAL:HA	1.97	0.44
1:E:233:GLY:O	1:E:235:ASN:ND2	2.49	0.44
1:G:75:VAL:HG13	1:G:76:ARG:HG2	1.98	0.44
1:G:77:PRO:O	2:M:280:GLY:HA3	2.18	0.44
1:G:167:VAL:HG12	1:G:167:VAL:O	2.17	0.44
1:D:193:PHE:CE1	3:N:286:SER:HB2	2.53	0.44
1:H:211:THR:HG23	1:H:217:ILE:HD11	1.98	0.44
1:B:89:ALA:HB2	1:B:146:VAL:HA	1.98	0.44
1:D:197:ALA:HB3	3:N:259:LEU:HB2	2.00	0.44
1:G:198:GLN:NE2	2:M:258:ASN:OD1	2.46	0.44
1:H:40:LEU:HD23	1:H:40:LEU:HA	1.87	0.44
1:F:106:GLN:HB2	1:F:112:TYR:CD1	2.53	0.44
1:F:195:PRO:HD2	3:O:261:ALA:HB2	1.98	0.44
1:B:81:ASP:O	1:B:243:LYS:NZ	2.51	0.44
1:E:148:MET:HG3	1:E:241:LEU:HG	2.00	0.44
1:H:143:TYR:CE2	1:H:145:ARG:HB2	2.53	0.44
1:B:106:GLN:HB2	1:B:112:TYR:CE2	2.52	0.44
1:E:52:ALA:HA	1:E:71:LEU:HA	2.00	0.44
1:A:86:VAL:HG22	2:I:279:ILE:O	2.18	0.44
1:E:165:PHE:O	1:E:204:THR:N	2.51	0.43
1:A:99:ILE:HG23	1:A:131:GLY:N	2.32	0.43
1:B:143:TYR:CZ	1:B:145:ARG:HB2	2.53	0.43
1:C:180:ALA:O	1:C:184:ARG:NH2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:ARG:HA	1:G:249:ARG:HA	2.00	0.43
1:A:219:PRO:HG3	1:A:221:ARG:NH1	2.33	0.43
1:A:134:VAL:HG12	2:I:258:ASN:HB2	2.00	0.43
1:B:168:ASN:OD1	1:B:168:ASN:N	2.49	0.43
1:B:235:ASN:H	1:B:238:SER:HB3	1.83	0.43
3:N:273:SER:HB2	3:N:274:LEU:HD22	1.99	0.43
1:H:206:VAL:CG1	1:H:250:PHE:HB3	2.49	0.43
1:D:64:ASN:OD1	1:D:252:LEU:HB2	2.17	0.43
1:A:26:ALA:HB1	1:A:63:PHE:HB3	2.01	0.43
1:D:38:ILE:HG12	1:D:66:PHE:CD2	2.53	0.43
1:G:186:ILE:HG23	1:G:199:ILE:HG12	2.00	0.43
3:N:267:LEU:HA	3:N:284:ALA:HA	2.01	0.43
1:E:106:GLN:HB2	1:E:112:TYR:CD2	2.54	0.43
1:G:193:PHE:CE2	2:M:286:SER:HB2	2.54	0.43
1:A:81:ASP:O	1:A:84:VAL:HG22	2.19	0.43
1:E:72:ARG:O	1:E:75:VAL:HG12	2.18	0.43
1:A:42:VAL:HA	1:A:47:VAL:HG23	1.99	0.42
1:H:199:ILE:HD12	3:P:257:ILE:HD11	2.01	0.42
1:A:143:TYR:CZ	1:A:145:ARG:HB2	2.55	0.42
1:F:13:LEU:O	1:F:15:LYS:HD3	2.18	0.42
1:F:86:VAL:HB	1:F:243:LYS:HE3	2.01	0.42
1:E:33:LEU:H	1:E:33:LEU:HD12	1.84	0.42
1:B:166:SER:N	1:B:204:THR:HB	2.35	0.42
1:B:179:PHE:CE1	2:J:255:THR:HG21	2.54	0.42
1:E:165:PHE:H	1:E:182:ASN:ND2	2.11	0.42
2:I:273:SER:HB2	2:I:274:LEU:HD22	2.02	0.42
1:B:51:GLU:HG2	1:B:75:VAL:HG21	2.01	0.42
1:H:168:ASN:ND2	1:H:170:LEU:HB2	2.35	0.42
1:C:87:MET:HA	2:K:283:LEU:HD22	2.01	0.42
1:G:88:PRO:HG3	2:M:258:ASN:HD21	1.85	0.42
1:H:93:ILE:HD12	3:P:275:SER:HB2	2.02	0.42
1:H:146:VAL:HG21	3:P:256:VAL:HG11	2.02	0.42
1:A:159:TYR:OH	1:A:183:GLU:OE2	2.31	0.42
1:A:162:GLY:HA3	1:A:181:ARG:O	2.20	0.42
1:C:9:LEU:O	1:C:13:LEU:HB2	2.20	0.42
1:H:34:THR:O	1:H:38:ILE:HG13	2.20	0.42
1:A:205:ILE:HG21	1:A:205:ILE:HD13	1.75	0.42
1:B:96:LEU:HD12	2:J:267:LEU:HD22	2.02	0.42
1:B:148:MET:HG3	1:B:241:LEU:HG	2.00	0.42
1:D:10:GLN:HE21	1:D:10:GLN:HB3	1.65	0.42
1:D:159:TYR:HB3	1:D:226:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ASN:OD1	1:D:168:ASN:N	2.53	0.42
1:G:219:PRO:HG3	1:G:221:ARG:HH12	1.85	0.42
1:H:211:THR:HA	1:H:248:GLY:HA2	2.01	0.42
1:B:1:MET:O	1:B:4:SER:HB2	2.20	0.41
1:B:87:MET:HA	2:J:283:LEU:HD22	2.00	0.41
1:H:13:LEU:O	1:H:15:LYS:NZ	2.48	0.41
1:H:177:ASN:HB3	1:H:180:ALA:HB3	2.01	0.41
1:A:15:LYS:O	1:A:19:THR:OG1	2.37	0.41
1:C:42:VAL:HG13	1:C:47:VAL:HB	2.02	0.41
1:F:4:SER:HA	1:F:7:LEU:HB2	2.01	0.41
1:H:137:TYR:CE1	1:H:167:VAL:HG13	2.55	0.41
1:A:76:ARG:HA	1:A:76:ARG:HD3	1.79	0.41
1:C:75:VAL:HG13	1:C:76:ARG:HG2	2.02	0.41
1:E:19:THR:HG22	1:E:205:ILE:HA	2.01	0.41
1:F:1:MET:O	1:F:4:SER:HB2	2.21	0.41
1:F:205:ILE:HD13	1:F:205:ILE:HA	1.91	0.41
1:A:7:LEU:HD23	1:A:7:LEU:H	1.85	0.41
1:B:195:PRO:HD2	2:J:261:ALA:HB2	2.02	0.41
1:C:199:ILE:O	2:K:256:VAL:HA	2.20	0.41
2:K:268:VAL:HB	2:K:271:LEU:HD12	2.02	0.41
1:D:241:LEU:HD11	1:D:247:MET:HB3	2.02	0.41
1:F:38:ILE:HG12	1:F:66:PHE:CD2	2.55	0.41
3:O:258:ASN:HB3	3:O:260:PHE:HE1	1.86	0.41
1:F:84:VAL:HA	3:O:285:VAL:HA	2.02	0.41
1:B:17:TRP:HA	1:B:17:TRP:CE3	2.55	0.41
1:C:29:ARG:HB3	1:C:62:THR:HG22	2.02	0.41
1:H:104:ILE:HD11	1:H:114:LEU:HD13	2.03	0.41
1:H:148:MET:HG3	1:H:241:LEU:HG	2.02	0.41
1:H:205:ILE:HD13	1:H:205:ILE:HA	1.91	0.41
1:D:12:ILE:HD12	1:D:12:ILE:HA	1.93	0.41
1:E:167:VAL:HA	1:E:178:LEU:HD21	2.03	0.41
1:G:99:ILE:HD11	1:G:128:PHE:O	2.21	0.41
1:G:250:PHE:CD2	2:M:254:PPI:H33	2.54	0.41
1:C:150:CYS:HA	1:C:243:LYS:HB2	2.03	0.41
1:D:3:ASN:O	1:D:7:LEU:HD13	2.21	0.41
1:D:86:VAL:HG12	1:D:149:PRO:O	2.21	0.41
1:E:143:TYR:OH	1:E:145:ARG:HB2	2.21	0.41
4:L:301:PEE:O1P	4:L:301:PEE:H12	2.20	0.41
1:F:233:GLY:HA2	1:F:238:SER:OG	2.21	0.41
1:G:4:SER:O	1:G:8:SER:OG	2.31	0.41
1:G:155:ARG:CZ	1:G:232:ALA:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:LEU:HD21	3:P:272:GLU:HA	2.03	0.41
1:G:91:GLY:HA2	1:G:142:ASP:OD2	2.21	0.40
1:H:210:GLU:HB3	1:H:216:THR:HA	2.03	0.40
1:A:99:ILE:O	1:A:130:ASN:HA	2.21	0.40
1:C:137:TYR:HE1	1:C:167:VAL:HG13	1.86	0.40
1:G:204:THR:HG21	4:M:301:PEE:H14	2.03	0.40
1:B:147:HIS:CD2	2:J:279:ILE:HD13	2.56	0.40
1:G:122:TYR:HA	1:G:125:ALA:HB3	2.03	0.40
1:G:159:TYR:OH	1:G:183:GLU:OE2	2.31	0.40
1:A:-1:ASP:HA	1:A:2:LEU:HB3	2.04	0.40
1:D:33:LEU:O	1:D:37:VAL:HG23	2.21	0.40
1:E:166:SER:O	4:L:301:PEE:O1P	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/267 (95%)	228 (90%)	25 (10%)	0	100	100
1	B	253/267 (95%)	229 (90%)	24 (10%)	0	100	100
1	C	253/267 (95%)	230 (91%)	23 (9%)	0	100	100
1	D	253/267 (95%)	228 (90%)	25 (10%)	0	100	100
1	E	253/267 (95%)	233 (92%)	19 (8%)	1 (0%)	34	71
1	F	253/267 (95%)	229 (90%)	23 (9%)	1 (0%)	34	71
1	G	253/267 (95%)	232 (92%)	20 (8%)	1 (0%)	34	71
1	H	253/267 (95%)	230 (91%)	23 (9%)	0	100	100
2	I	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
2	J	32/36 (89%)	28 (88%)	4 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
2	L	32/36 (89%)	28 (88%)	4 (12%)	0	100	100
2	M	31/36 (86%)	29 (94%)	2 (6%)	0	100	100
3	N	33/36 (92%)	29 (88%)	4 (12%)	0	100	100
3	O	33/36 (92%)	29 (88%)	4 (12%)	0	100	100
3	P	33/36 (92%)	29 (88%)	3 (9%)	1 (3%)	4	33
All	All	2282/2424 (94%)	2071 (91%)	207 (9%)	4 (0%)	47	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	255	THR
1	E	167	VAL
1	F	88	PRO
1	G	206	VAL

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	216/229 (94%)	210 (97%)	6 (3%)	43	72
1	B	215/229 (94%)	207 (96%)	8 (4%)	34	66
1	C	209/229 (91%)	203 (97%)	6 (3%)	42	72
1	D	214/229 (93%)	205 (96%)	9 (4%)	30	63
1	E	211/229 (92%)	201 (95%)	10 (5%)	26	61
1	F	213/229 (93%)	207 (97%)	6 (3%)	43	72
1	G	215/229 (94%)	209 (97%)	6 (3%)	43	72
1	H	209/229 (91%)	205 (98%)	4 (2%)	57	80
2	I	27/31 (87%)	26 (96%)	1 (4%)	34	66
2	J	27/31 (87%)	27 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	27/31 (87%)	27 (100%)	0	100	100
2	L	27/31 (87%)	27 (100%)	0	100	100
2	M	27/31 (87%)	27 (100%)	0	100	100
3	N	27/31 (87%)	27 (100%)	0	100	100
3	O	27/31 (87%)	27 (100%)	0	100	100
3	P	26/31 (84%)	26 (100%)	0	100	100
All	All	1917/2080 (92%)	1861 (97%)	56 (3%)	42	72

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	20	ARG
1	A	29	ARG
1	A	41	PHE
1	A	113	SER
1	A	236	ASP
2	I	264	LYS
1	B	20	ARG
1	B	33	LEU
1	B	69	ARG
1	B	73	ASP
1	B	164	LEU
1	B	218	THR
1	B	236	ASP
1	B	238	SER
1	C	20	ARG
1	C	53	GLN
1	C	69	ARG
1	C	113	SER
1	C	139	SER
1	C	182	ASN
1	D	1	MET
1	D	13	LEU
1	D	20	ARG
1	D	32	TRP
1	D	66	PHE
1	D	69	ARG
1	D	143	TYR
1	D	173	GLN

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Mol	Chain	Res	Type
1	D	236	ASP
1	E	-1	ASP
1	E	5	PHE
1	E	11	TYR
1	E	13	LEU
1	E	20	ARG
1	E	66	PHE
1	E	69	ARG
1	E	122	TYR
1	E	143	TYR
1	E	236	ASP
1	F	5	PHE
1	F	15	LYS
1	F	20	ARG
1	F	66	PHE
1	F	143	TYR
1	F	182	ASN
1	G	20	ARG
1	G	29	ARG
1	G	69	ARG
1	G	73	ASP
1	G	151	ASN
1	G	236	ASP
1	H	1	MET
1	H	20	ARG
1	H	69	ARG
1	H	96	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	147	HIS
1	E	168	ASN
1	G	198	GLN
2	M	258	ASN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#|Z| > 2$
4	PEE	J	301	2	22,22,50	1.41	2 (9%)	25,27,55	1.23	3 (12%)
4	PEE	K	301	2	22,22,50	1.41	2 (9%)	25,27,55	1.14	3 (12%)
4	PEE	M	301	2	22,22,50	1.39	2 (9%)	25,27,55	1.11	2 (8%)
4	PEE	I	301	2	22,22,50	1.41	2 (9%)	25,27,55	1.38	4 (16%)
4	PEE	L	301	2	22,22,50	1.45	2 (9%)	25,27,55	1.33	3 (12%)

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
4	PEE	J	301	2	-	11/26/26/54	-
4	PEE	K	301	2	-	11/26/26/54	-
4	PEE	M	301	2	-	11/26/26/54	-
4	PEE	I	301	2	-	13/26/26/54	-
4	PEE	L	301	2	-	11/26/26/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	301	PEE	O2-C10	4.67	1.47	1.34
4	I	301	PEE	O2-C10	4.45	1.46	1.34
4	J	301	PEE	O2-C10	4.42	1.46	1.34
4	K	301	PEE	O2-C10	4.42	1.46	1.34
4	M	301	PEE	O2-C10	4.34	1.46	1.34
4	L	301	PEE	O3-C30	4.33	1.46	1.33
4	K	301	PEE	O3-C30	4.23	1.45	1.33
4	J	301	PEE	O3-C30	4.23	1.45	1.33
4	M	301	PEE	O3-C30	4.20	1.45	1.33
4	I	301	PEE	O3-C30	4.00	1.45	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	301	PEE	O2-C10-C11	4.56	121.33	111.50
4	J	301	PEE	O2-C10-C11	3.83	119.76	111.50
4	L	301	PEE	O2-C10-C11	3.82	119.74	111.50
4	M	301	PEE	O2-C10-C11	3.34	118.70	111.50
4	K	301	PEE	O2-C10-C11	3.25	118.51	111.50
4	L	301	PEE	C3-C2-C1	-3.01	104.66	111.79
4	L	301	PEE	O3-C30-C31	2.80	120.70	111.91
4	J	301	PEE	O3-C30-C31	2.53	119.85	111.91
4	K	301	PEE	O3-C30-C31	2.51	119.80	111.91
4	I	301	PEE	C3-O3-C30	2.40	126.01	117.12
4	M	301	PEE	O3-C30-C31	2.28	119.06	111.91
4	I	301	PEE	O3-C30-C31	2.14	118.63	111.91
4	J	301	PEE	O3-C30-O5	-2.11	118.26	123.59
4	K	301	PEE	O3-C30-O5	-2.06	118.40	123.59
4	I	301	PEE	O3-C3-C2	2.01	114.28	108.43

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	301	PEE	O2-C2-C3-O3
4	I	301	PEE	C1-O3P-P-O2P
4	I	301	PEE	C1-O3P-P-O1P
4	I	301	PEE	C4-O4P-P-O2P
4	J	301	PEE	C11-C10-O2-C2
4	M	301	PEE	C2-C1-O3P-P
4	L	301	PEE	C2-C3-O3-C30
4	J	301	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
4	K	301	PEE	O5-C30-O3-C3
4	L	301	PEE	O5-C30-O3-C3
4	J	301	PEE	O4-C10-O2-C2
4	J	301	PEE	C31-C30-O3-C3
4	L	301	PEE	C31-C30-O3-C3
4	K	301	PEE	C31-C30-O3-C3
4	K	301	PEE	C2-C3-O3-C30
4	J	301	PEE	C2-C1-O3P-P
4	I	301	PEE	C11-C10-O2-C2
4	I	301	PEE	C1-O3P-P-O4P
4	I	301	PEE	C4-O4P-P-O3P
4	M	301	PEE	C1-O3P-P-O4P
4	I	301	PEE	O4-C10-O2-C2
4	M	301	PEE	O4-C10-O2-C2
4	M	301	PEE	C11-C10-O2-C2
4	K	301	PEE	C11-C10-O2-C2
4	K	301	PEE	O4-C10-O2-C2
4	L	301	PEE	C4-O4P-P-O3P
4	I	301	PEE	C2-C1-O3P-P
4	M	301	PEE	C1-C2-O2-C10
4	I	301	PEE	C1-C2-C3-O3
4	J	301	PEE	C1-C2-O2-C10
4	M	301	PEE	O2-C2-C3-O3
4	I	301	PEE	C30-C31-C32-C33
4	K	301	PEE	C10-C11-C12-C13
4	L	301	PEE	C4-O4P-P-O2P
4	M	301	PEE	C1-O3P-P-O1P
4	I	301	PEE	C2-C3-O3-C30
4	J	301	PEE	O4P-C4-C5-N
4	L	301	PEE	C5-C4-O4P-P
4	M	301	PEE	C1-C2-C3-O3
4	K	301	PEE	C3-C2-O2-C10
4	J	301	PEE	C1-O3P-P-O4P
4	K	301	PEE	C2-C1-O3P-P
4	J	301	PEE	C10-C11-C12-C13
4	K	301	PEE	O2-C2-C3-O3
4	L	301	PEE	C1-C2-O2-C10
4	K	301	PEE	O4P-C4-C5-N
4	M	301	PEE	O4P-C4-C5-N
4	L	301	PEE	C10-C11-C12-C13
4	L	301	PEE	C3-C2-O2-C10
4	J	301	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
4	J	301	PEE	C4-O4P-P-O1P
4	K	301	PEE	C4-O4P-P-O1P
4	L	301	PEE	C1-O3P-P-O1P
4	L	301	PEE	C4-O4P-P-O1P
4	I	301	PEE	C5-C4-O4P-P
4	M	301	PEE	C5-C4-O4P-P
4	M	301	PEE	O3-C30-C31-C32

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	301	PEE	1	0
4	K	301	PEE	3	0
4	M	301	PEE	3	0
4	I	301	PEE	7	0
4	L	301	PEE	5	0

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

Ligand PEE J 301

Bond lengths

Bond angles

Torsions

Rings

Ligand PEE K 301

Bond lengths

Bond angles

Torsions

Rings

Ligand PEE M 301

Bond lengths

Bond angles

Torsions

Rings

Ligand PEE I 301

Bond lengths

Bond angles

Torsions

Rings

Ligand PEE L 301

Bond lengths

Bond angles

Torsions

Rings
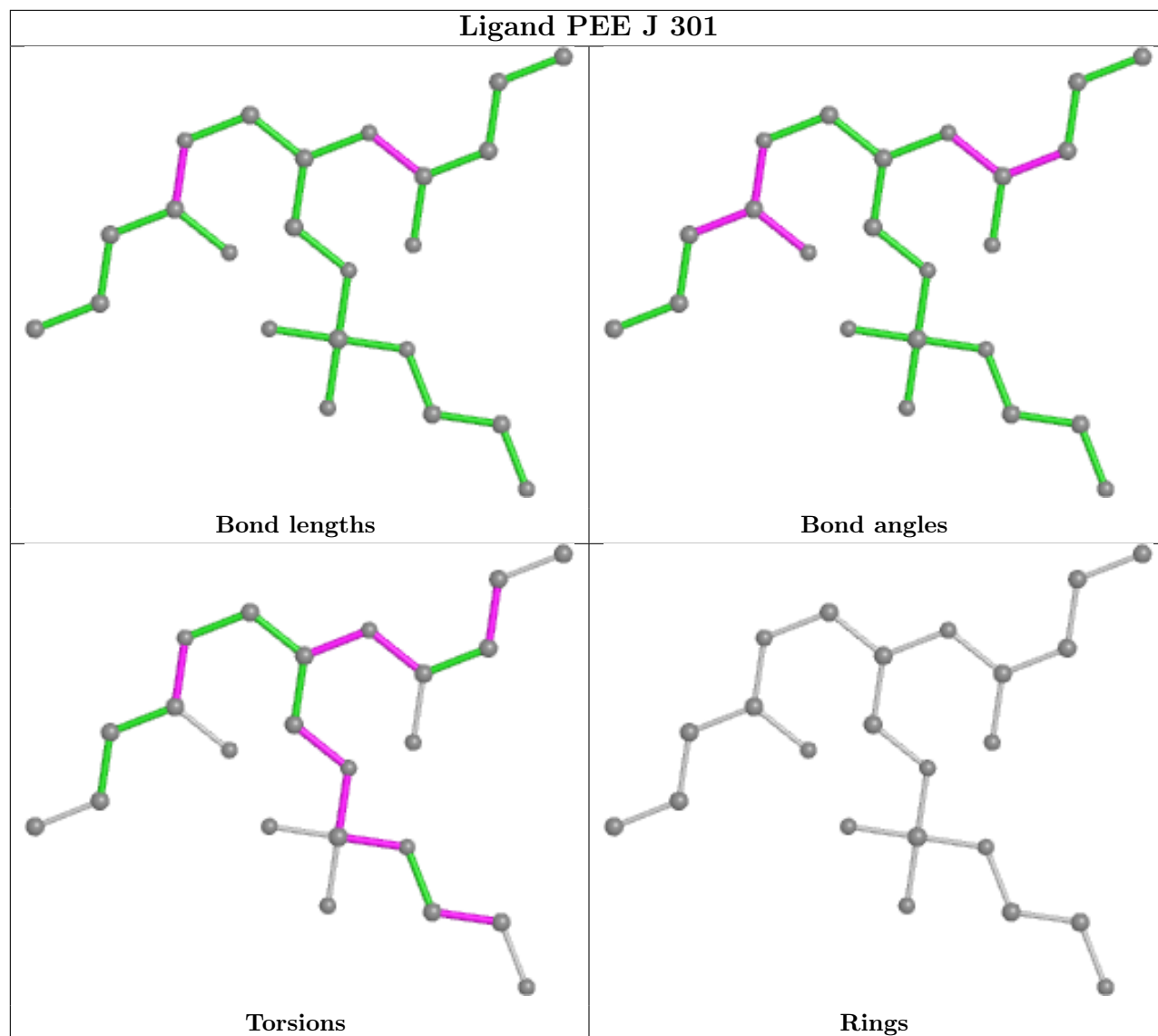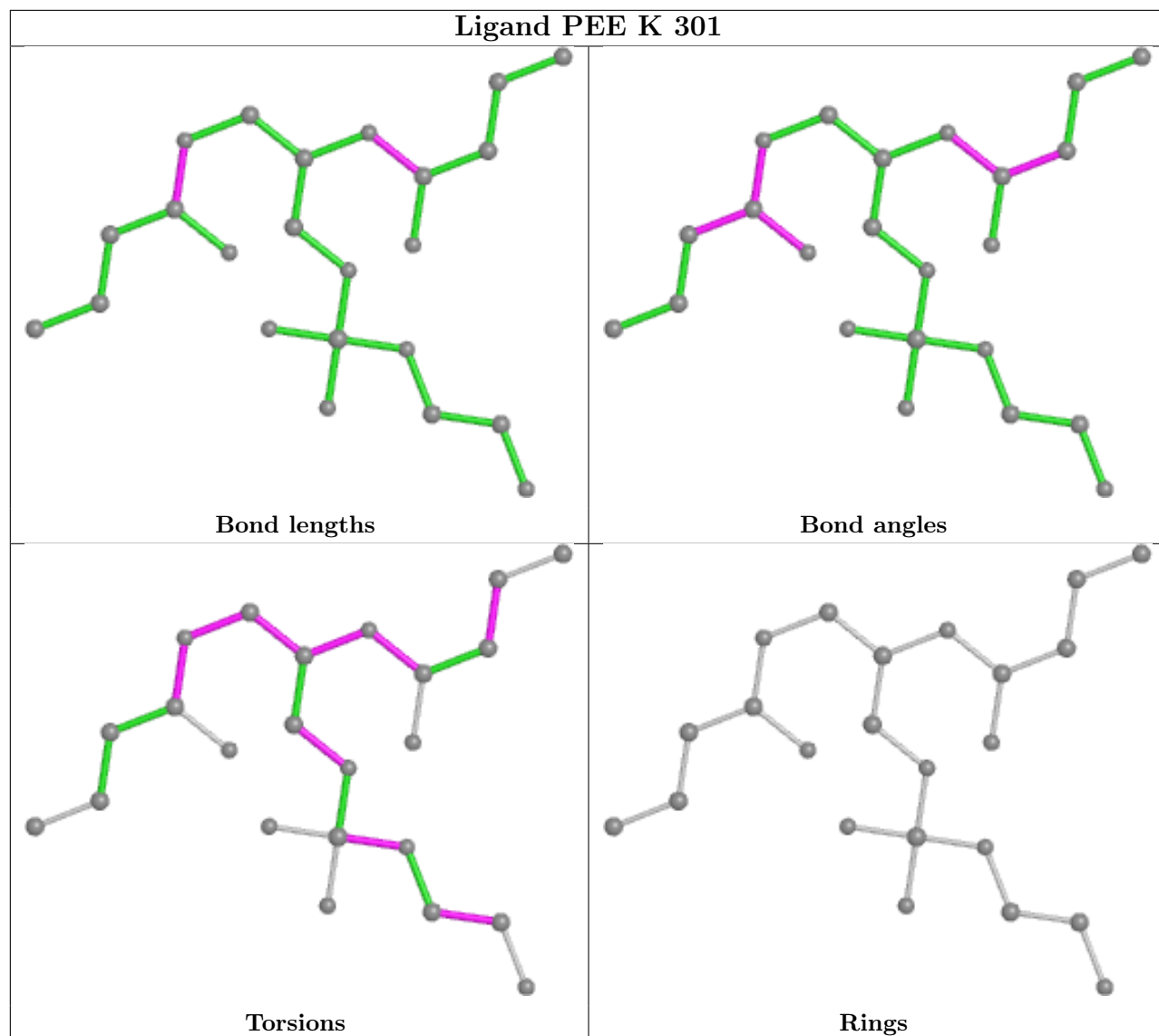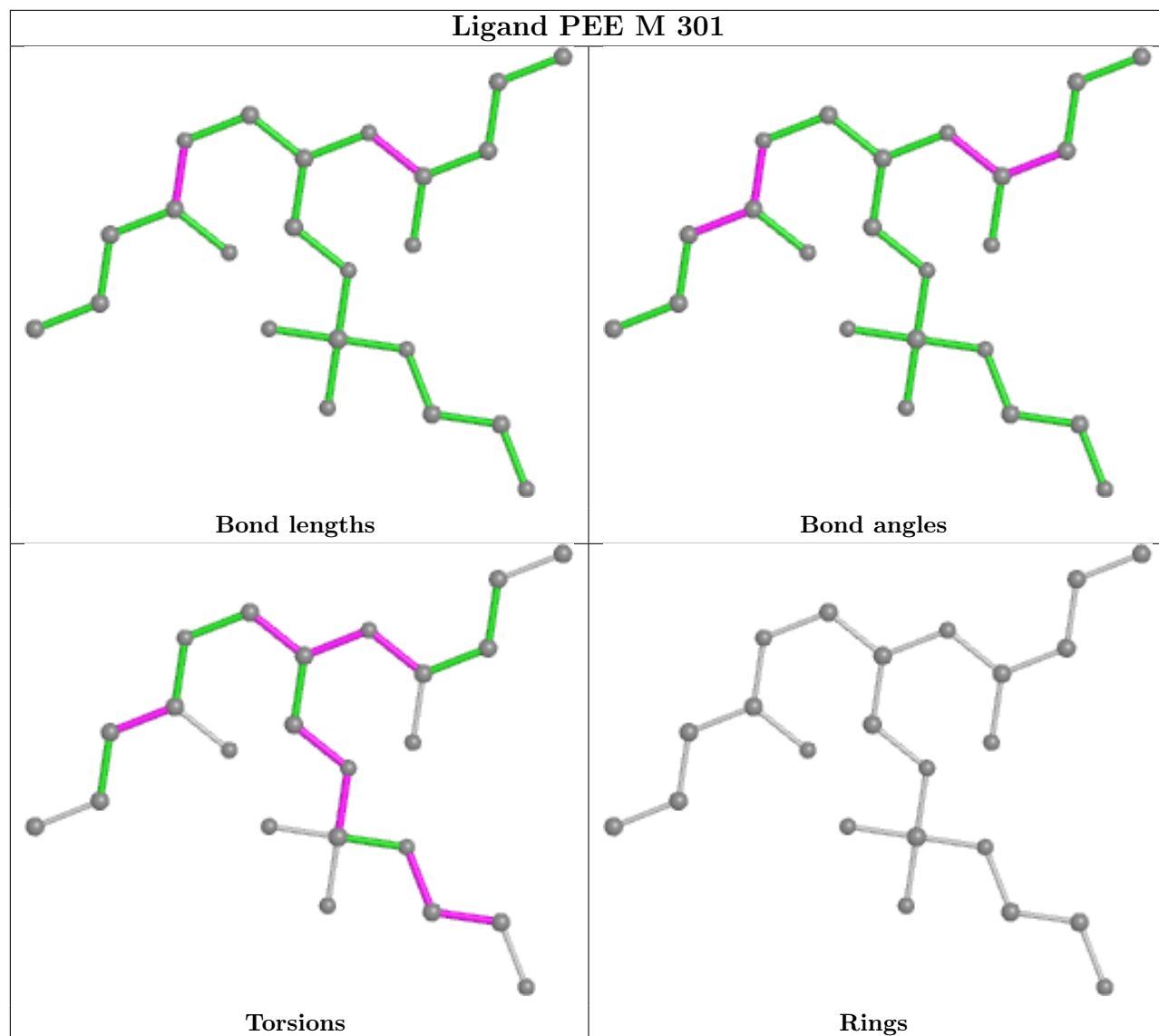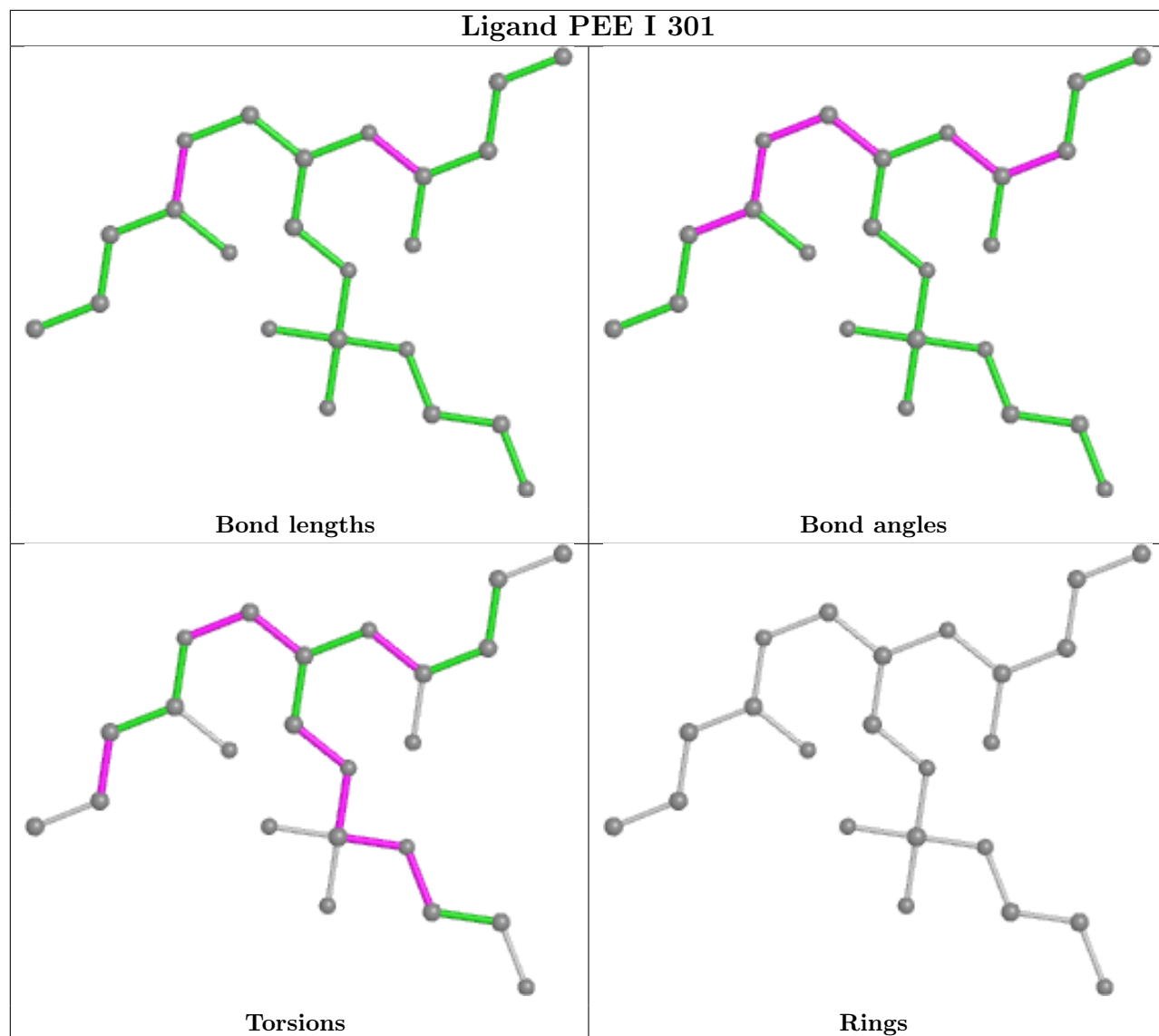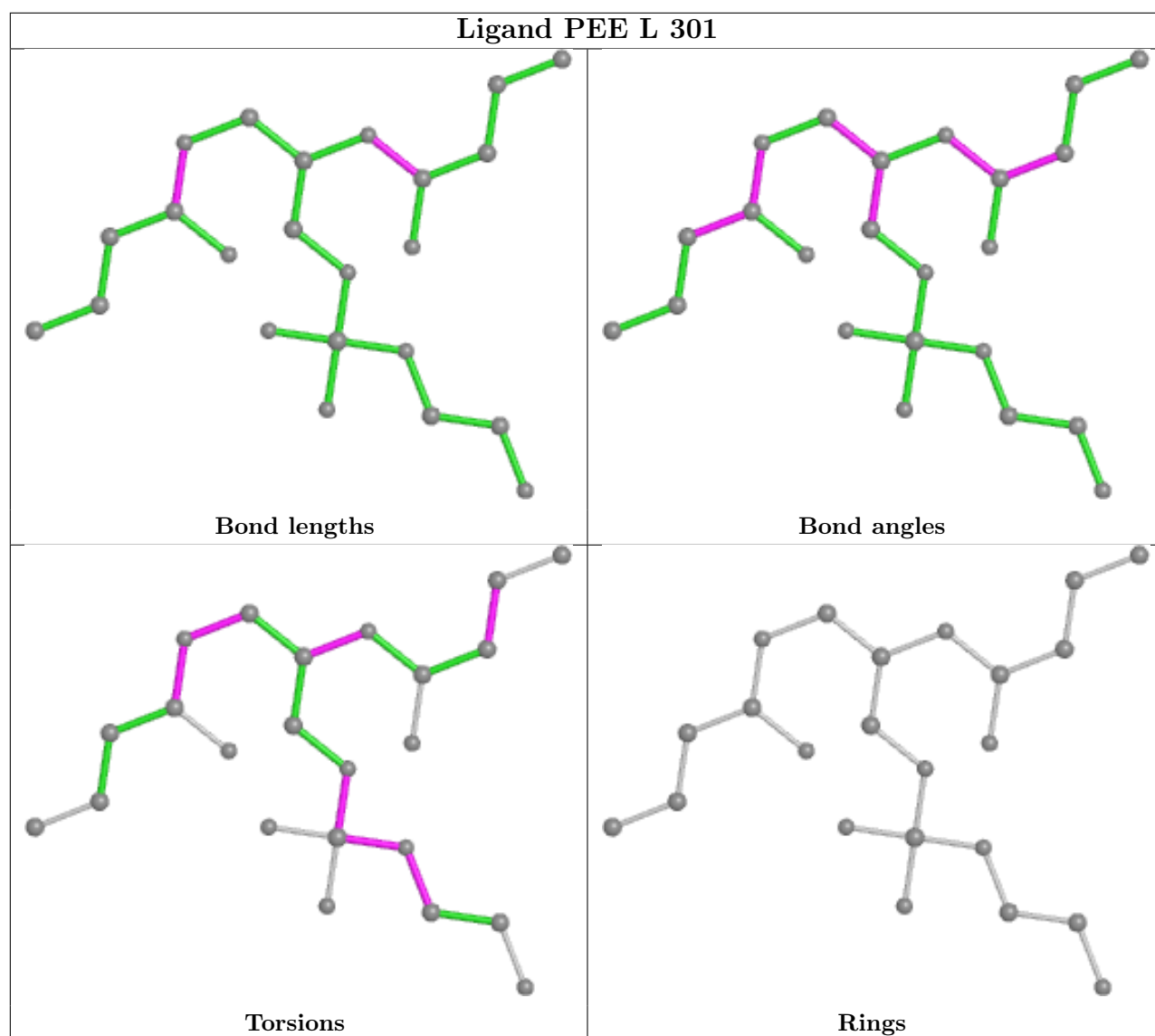
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	255/267 (95%)	-0.33	0	100	100	106, 129, 165, 190	0
1	B	255/267 (95%)	-0.35	0	100	100	106, 137, 170, 196	0
1	C	255/267 (95%)	-0.29	0	100	100	115, 140, 177, 198	0
1	D	255/267 (95%)	-0.31	1 (0%)	92	86	108, 144, 181, 209	0
1	E	255/267 (95%)	-0.30	4 (1%)	72	57	119, 156, 184, 194	0
1	F	255/267 (95%)	-0.34	0	100	100	131, 160, 184, 195	0
1	G	255/267 (95%)	-0.19	3 (1%)	79	66	121, 162, 187, 210	0
1	H	255/267 (95%)	0.20	17 (6%)	17	10	152, 189, 214, 226	0
2	I	34/36 (94%)	-0.13	0	100	100	104, 127, 146, 157	0
2	J	34/36 (94%)	-0.15	0	100	100	118, 145, 160, 173	0
2	K	34/36 (94%)	-0.47	0	100	100	128, 157, 182, 192	0
2	L	34/36 (94%)	-0.53	0	100	100	136, 168, 184, 195	0
2	M	33/36 (91%)	-0.01	0	100	100	150, 179, 193, 196	0
3	N	34/36 (94%)	-0.17	1 (2%)	51	35	125, 155, 170, 172	0
3	O	34/36 (94%)	0.04	1 (2%)	51	35	143, 166, 176, 183	0
3	P	34/36 (94%)	0.40	5 (14%)	2	1	180, 205, 218, 222	0
All	All	2311/2424 (95%)	-0.23	32 (1%)	75	61	104, 153, 199, 226	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	196	MET	6.6
1	H	187	CYS	4.8
1	H	189	PHE	4.8
3	P	260	PHE	4.6
1	H	195	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	149	PRO	3.6
1	H	188	LEU	3.4
1	H	198	GLN	3.3
1	H	148	MET	3.3
3	P	259	LEU	3.2
3	P	288	GLU	3.1
1	H	197	ALA	3.1
1	H	61	ARG	3.1
3	P	258	ASN	2.8
1	H	86	VAL	2.8
1	G	179	PHE	2.7
1	H	85	LEU	2.6
3	O	259	LEU	2.6
1	G	209	ILE	2.6
1	D	135	THR	2.3
3	N	282	PRO	2.3
1	E	187	CYS	2.3
1	H	63	PHE	2.2
1	E	157	MET	2.2
1	H	194	GLY	2.1
1	E	221	ARG	2.1
1	E	202	GLY	2.1
1	H	154	LEU	2.1
1	G	252	LEU	2.1
1	H	66	PHE	2.1
3	P	279	ILE	2.0
1	H	57	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEE	L	301	23/51	0.89	0.27	109,142,164,167	0
4	PEE	I	301	23/51	0.90	0.29	106,142,148,155	0
4	PEE	M	301	23/51	0.90	0.26	129,148,161,168	0
4	PEE	J	301	23/51	0.93	0.25	110,138,150,158	0
4	PEE	K	301	23/51	0.93	0.31	105,130,143,156	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.
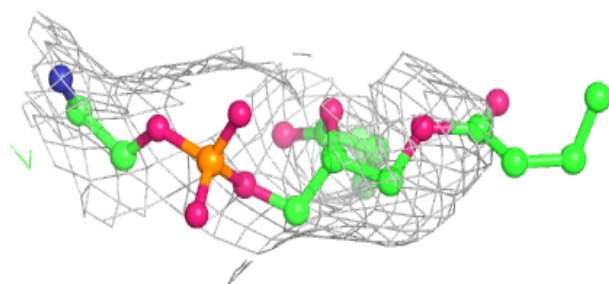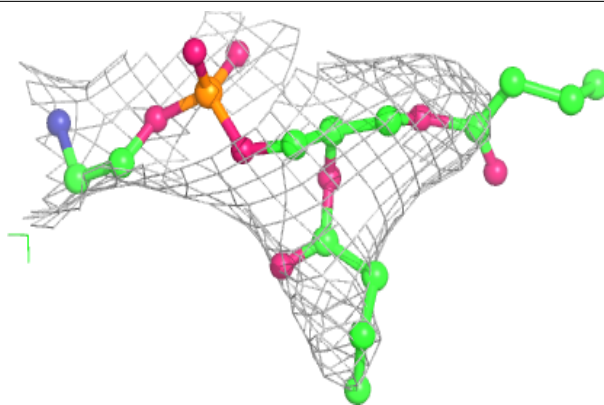

Electron density around PEE L 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
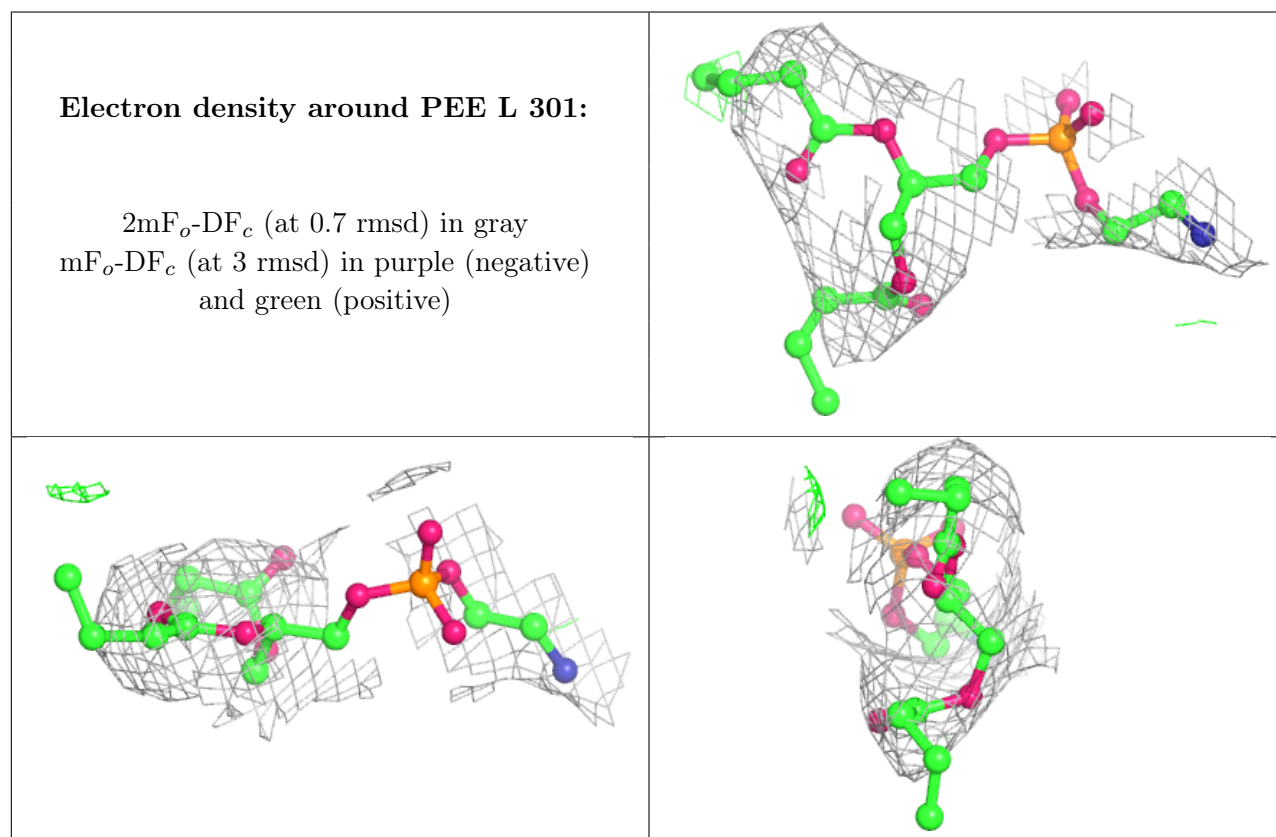
Electron density around PEE I 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
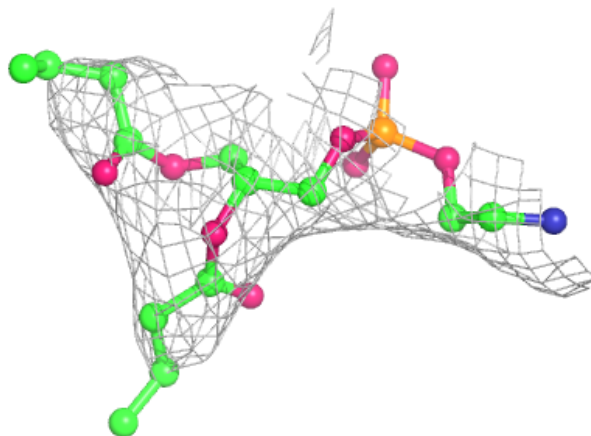and green (positive)
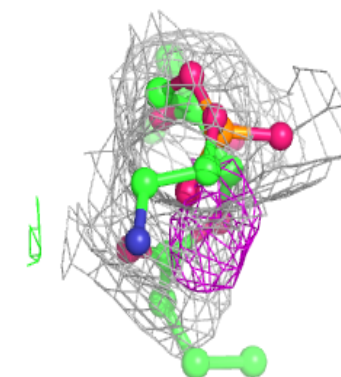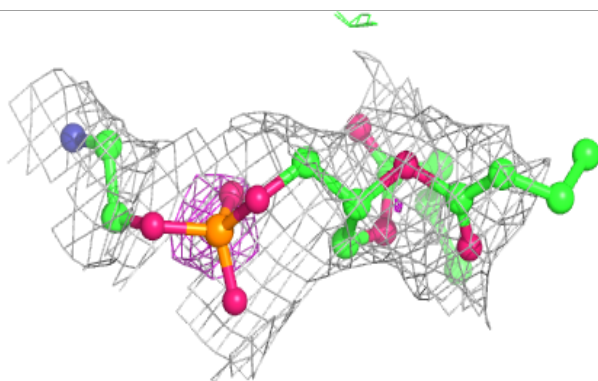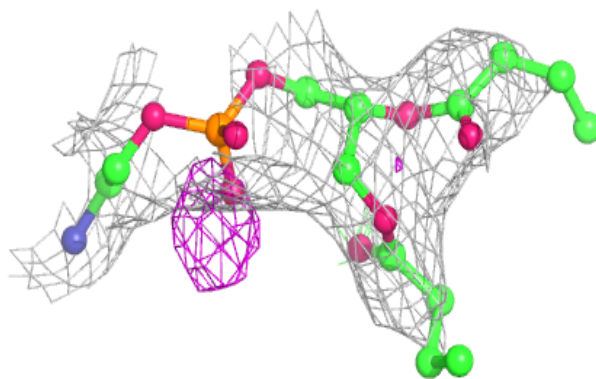
Electron density around PEE M 301:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
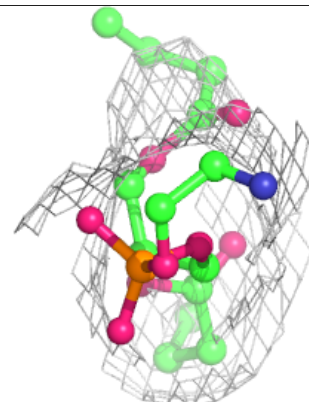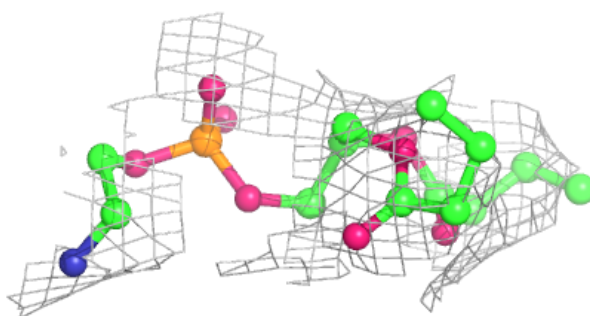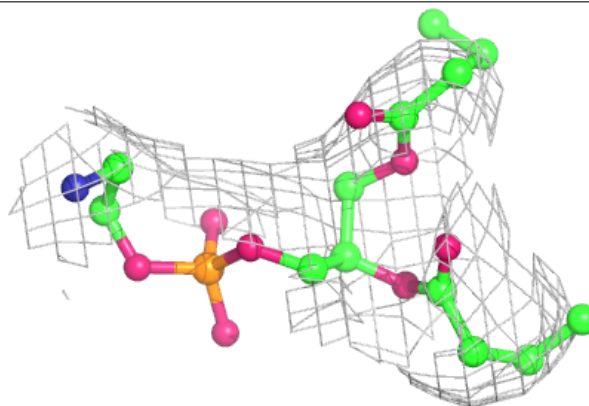
Electron density around PEE J 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
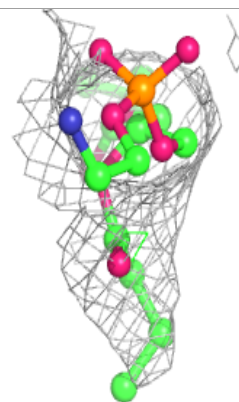
Electron density around PEE K 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
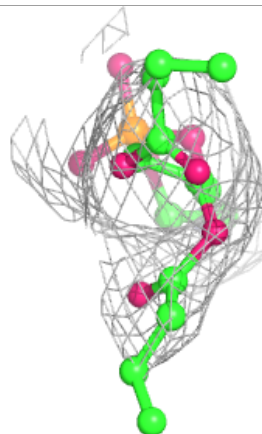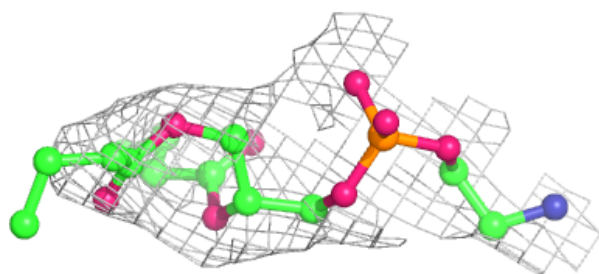
6.5 Other polymers (i)

There are no such residues in this entry.