



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:14 am BST

PDB ID : 5GYK
Title : Crystal Structure of Mdm12-deletion mutant
Authors : Jeong, H.; Park, J.; Lee, C.
Deposited on : 2016-09-22
Resolution : 3.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

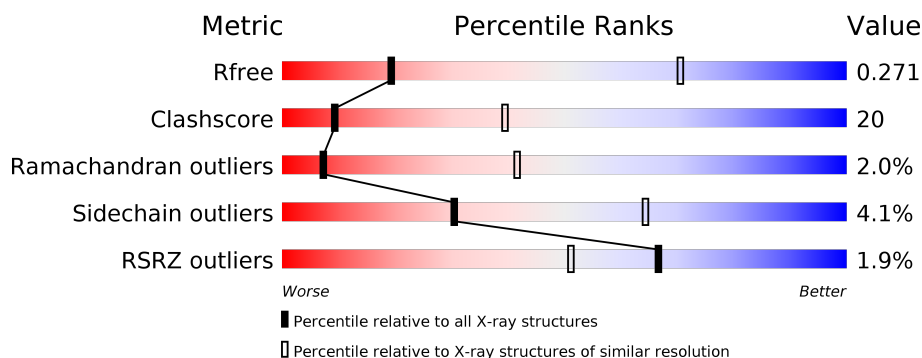
1 Overall quality at a glance

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	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 on 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	236	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>24%</div> <div>5%</div> <div>• •</div> </div> </div>
1	B	236	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>•</div> <div>6%</div> </div> </div>
1	C	236	<div> <div></div> <div> <div></div> <div>67%</div> <div>27%</div> <div>• •</div> </div> </div>
1	D	236	<div> <div></div> <div> <div></div> <div>71%</div> <div>22%</div> <div>• •</div> </div> </div>
1	E	236	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>5%</div> <div>•</div> </div> </div>
1	F	236	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>30%</div> <div>• •</div> <div>5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEE	A	301	-	-	-	X
2	PEE	D	301	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10874 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 Mitochondrial distribution and morphology protein 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1814	1168	290	350	6			
1	B	223	Total	C	N	O	S	0	0	0
			1778	1146	285	341	6			
1	C	226	Total	C	N	O	S	0	0	0
			1805	1163	289	347	6			
1	D	227	Total	C	N	O	S	0	0	0
			1814	1168	290	350	6			
1	E	226	Total	C	N	O	S	0	0	0
			1806	1164	288	348	6			
1	F	225	Total	C	N	O	S	0	0	0
			1795	1155	287	347	6			

There are 36 discrepancies between the modelled and reference sequences:

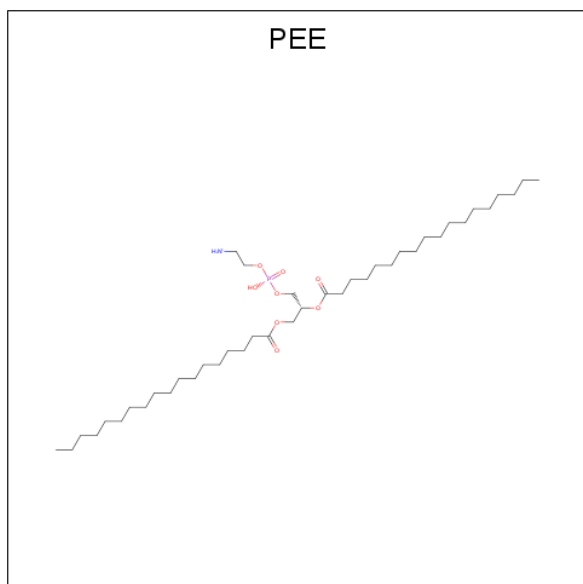
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q92328
A	110	GLY	-	linker	UNP Q92328
A	111	GLY	-	linker	UNP Q92328
A	112	SER	-	linker	UNP Q92328
A	113	GLY	-	linker	UNP Q92328
A	114	GLY	-	linker	UNP Q92328
B	0	GLY	-	expression tag	UNP Q92328
B	110	GLY	-	linker	UNP Q92328
B	111	GLY	-	linker	UNP Q92328
B	112	SER	-	linker	UNP Q92328
B	113	GLY	-	linker	UNP Q92328
B	114	GLY	-	linker	UNP Q92328
C	0	GLY	-	expression tag	UNP Q92328
C	110	GLY	-	linker	UNP Q92328
C	111	GLY	-	linker	UNP Q92328
C	112	SER	-	linker	UNP Q92328
C	113	GLY	-	linker	UNP Q92328

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Chain	Residue	Modelled	Actual	Comment	Reference
C	114	GLY	-	linker	UNP Q92328
D	0	GLY	-	expression tag	UNP Q92328
D	110	GLY	-	linker	UNP Q92328
D	111	GLY	-	linker	UNP Q92328
D	112	SER	-	linker	UNP Q92328
D	113	GLY	-	linker	UNP Q92328
D	114	GLY	-	linker	UNP Q92328
E	0	GLY	-	expression tag	UNP Q92328
E	110	GLY	-	linker	UNP Q92328
E	111	GLY	-	linker	UNP Q92328
E	112	SER	-	linker	UNP Q92328
E	113	GLY	-	linker	UNP Q92328
E	114	GLY	-	linker	UNP Q92328
F	0	GLY	-	expression tag	UNP Q92328
F	110	GLY	-	linker	UNP Q92328
F	111	GLY	-	linker	UNP Q92328
F	112	SER	-	linker	UNP Q92328
F	113	GLY	-	linker	UNP Q92328
F	114	GLY	-	linker	UNP Q92328

- Molecule 2 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₈₃NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	21	1	8	1		

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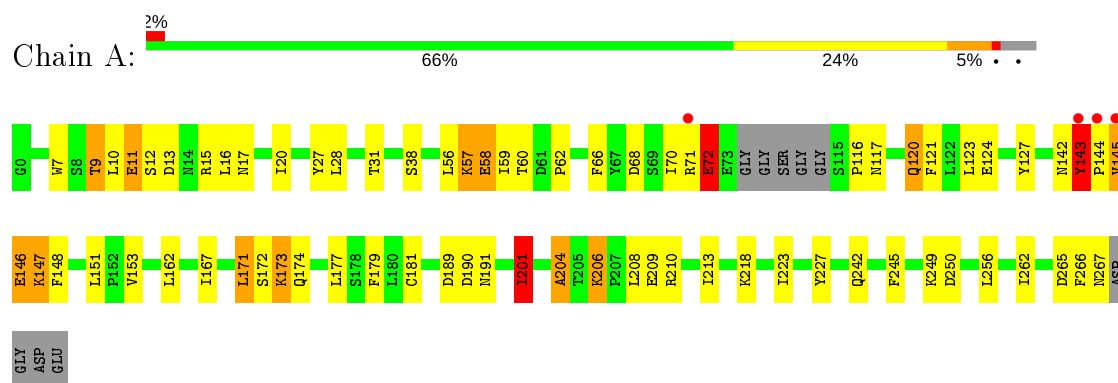
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			31	21	1	8	1		

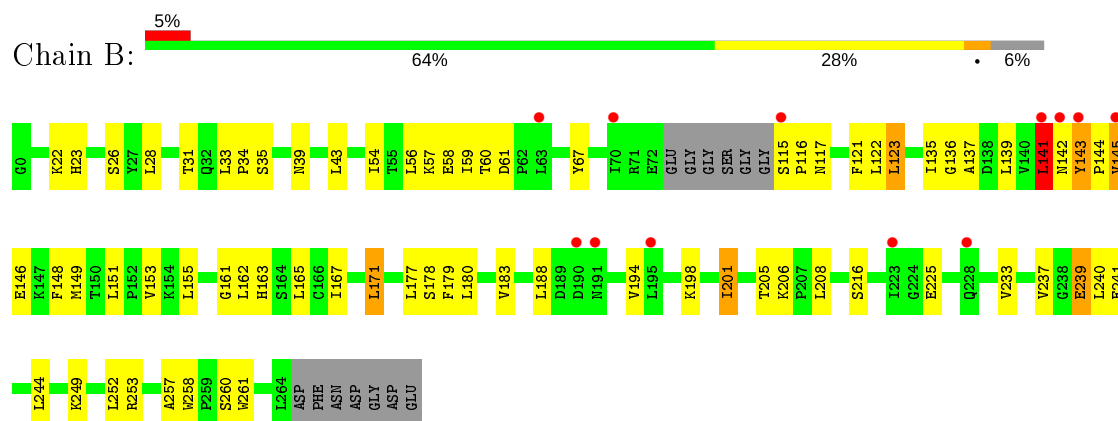
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

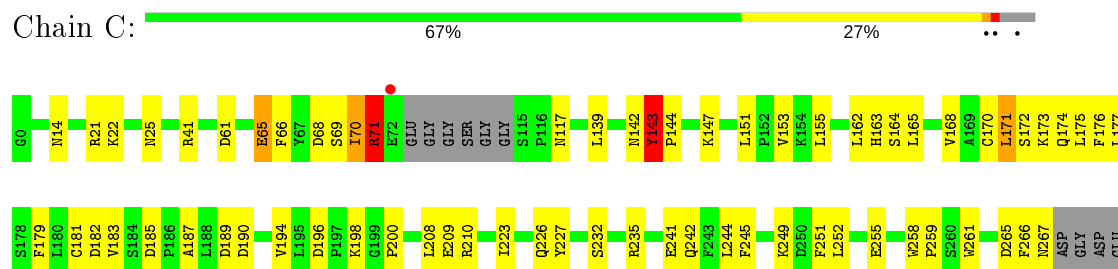
- Molecule 1: Mitochondrial distribution and morphology protein 12



- Molecule 1: Mitochondrial distribution and morphology protein 12

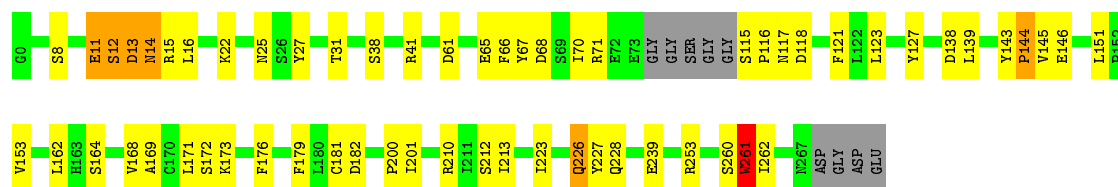


- Molecule 1: Mitochondrial distribution and morphology protein 12



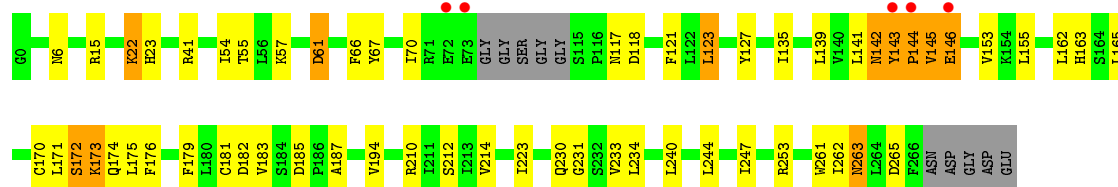
- Molecule 1: Mitochondrial distribution and morphology protein 12

Chain D:  71% 22% . .



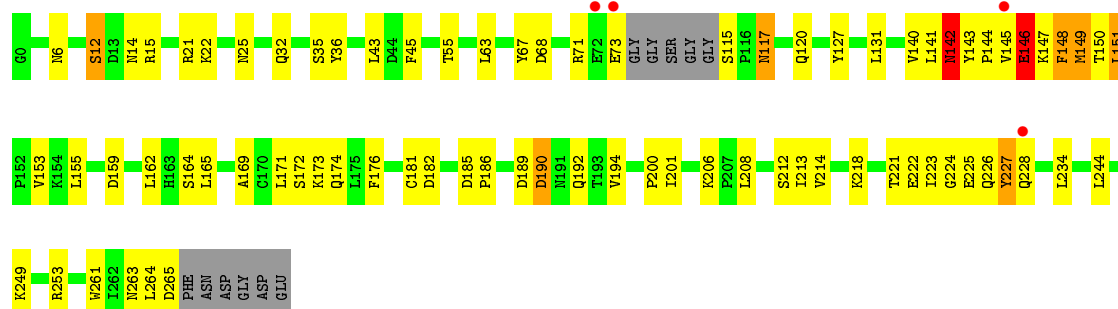
- Molecule 1: Mitochondrial distribution and morphology protein 12

Chain E:  2% 70% 21% 5% .



- Molecule 1: Mitochondrial distribution and morphology protein 12

Chain F:  2% 62% 30% 5% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.24Å 148.24Å 212.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.45 – 3.60 41.45 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.45-3.60) 89.7 (41.45-3.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.220 , 0.267 0.234 , 0.271	Depositor DCC
R_{free} test set	2000 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10874	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.42% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.31	0/1849	0.56	0/2509
1	B	0.38	0/1812	0.65	2/2459 (0.1%)
1	C	0.38	0/1840	0.69	3/2497 (0.1%)
1	D	0.43	2/1849 (0.1%)	0.67	0/2509
1	E	0.32	0/1841	0.57	0/2498
1	F	0.36	0/1829	0.69	1/2482 (0.0%)
All	All	0.37	2/11020 (0.0%)	0.64	6/14954 (0.0%)

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	A	0	2
1	B	0	1
1	C	0	3
1	D	0	1
1	E	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	261	TRP	CE3-CZ3	-6.15	1.28	1.38
1	D	261	TRP	CB-CG	-6.11	1.39	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	TYR	C-N-CD	8.07	145.35	128.40
1	C	171	LEU	CA-CB-CG	6.25	129.68	115.30
1	F	208	LEU	CA-CB-CG	5.86	128.78	115.30
1	B	141	LEU	N-CA-C	5.50	125.85	111.00
1	B	171	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	C	14	ASN	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	71	ARG	Peptide
1	A	72	GLU	Peptide
1	B	115	SER	Peptide
1	C	142	ASN	Peptide
1	C	70	ILE	Peptide
1	C	71	ARG	Peptide
1	D	260	SER	Peptide
1	E	173	LYS	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	1814	0	1821	85	0
1	B	1778	0	1796	68	0
1	C	1805	0	1815	58	0
1	D	1814	0	1821	66	0
1	E	1806	0	1815	60	0
1	F	1795	0	1805	107	0
2	A	31	0	36	6	0
2	D	31	0	36	9	0
All	All	10874	0	10945	431	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 20.

All (431) 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:143:TYR:CD1	1:A:144:PRO:HD2	1.29	1.60
1:A:143:TYR:HD1	1:A:144:PRO:CD	1.34	1.38
1:F:140:VAL:CG2	1:F:145:VAL:H	1.42	1.30
1:F:226:GLN:O	1:F:228:GLN:N	1.64	1.30
1:E:143:TYR:HB2	1:E:144:PRO:CD	1.64	1.28
1:D:8:SER:O	1:D:12:SER:HA	1.32	1.27
1:F:140:VAL:HG21	1:F:145:VAL:N	1.50	1.26
1:F:143:TYR:HD1	1:F:145:VAL:CG2	1.57	1.16
1:F:142:ASN:HB2	1:F:148:PHE:HD2	1.03	1.14
1:E:143:TYR:HB2	1:E:144:PRO:HD2	1.34	1.08
1:F:143:TYR:CD1	1:F:145:VAL:HG23	1.89	1.07
1:F:143:TYR:CD1	1:F:145:VAL:CG2	2.37	1.07
1:F:226:GLN:O	1:F:228:GLN:HG2	1.55	1.06
1:A:143:TYR:CD1	1:A:144:PRO:CD	2.18	1.06
1:F:143:TYR:HD1	1:F:145:VAL:HG21	1.15	1.06
1:E:145:VAL:HG13	1:E:146:GLU:H	1.14	1.06
1:C:174:GLN:NE2	1:C:267:ASN:HD21	1.55	1.05
1:F:144:PRO:HA	1:F:145:VAL:CB	1.84	1.04
1:E:143:TYR:HB2	1:E:144:PRO:HD3	1.40	1.01
1:E:145:VAL:CG1	1:E:146:GLU:N	2.25	1.00
1:F:142:ASN:HB2	1:F:148:PHE:CD2	1.95	1.00
1:F:142:ASN:O	1:F:144:PRO:O	1.79	1.00
1:C:174:GLN:HE22	1:C:267:ASN:ND2	1.60	1.00
1:F:145:VAL:O	1:F:145:VAL:HG12	1.61	0.99
1:F:144:PRO:HA	1:F:145:VAL:HB	1.00	0.98
1:A:11:GLU:HB3	1:A:12:SER:HB2	1.46	0.97
1:F:144:PRO:CA	1:F:145:VAL:HB	1.94	0.96
1:C:174:GLN:HE22	1:C:267:ASN:HD21	1.01	0.96
1:E:145:VAL:CG1	1:E:146:GLU:H	1.79	0.95
1:F:226:GLN:C	1:F:228:GLN:H	1.60	0.95
1:E:143:TYR:CB	1:E:144:PRO:CD	2.44	0.93
1:F:200:PRO:HB3	1:F:206:LYS:HZ1	1.31	0.93
1:A:62:PRO:HA	1:A:120:GLN:HE21	1.30	0.93
1:D:8:SER:O	1:D:12:SER:CA	2.15	0.93
1:F:144:PRO:HB3	1:F:145:VAL:O	1.68	0.92
1:A:9:THR:OG1	1:B:56:LEU:O	1.87	0.91
1:F:224:GLY:O	1:F:227:TYR:CD2	2.25	0.90
1:F:144:PRO:HB2	1:F:147:LYS:H	1.34	0.89
1:F:140:VAL:HG21	1:F:145:VAL:H	0.73	0.89
1:E:142:ASN:HD22	1:E:142:ASN:H	1.20	0.88
1:A:11:GLU:CB	1:A:12:SER:HB2	2.04	0.88
1:A:143:TYR:HB2	1:A:144:PRO:HD3	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:TYR:N	1:B:144:PRO:HD2	1.90	0.86
1:F:212:SER:OG	1:F:253:ARG:NH2	2.08	0.86
1:A:58:GLU:HG3	1:A:59:ILE:H	1.40	0.86
1:A:12:SER:HB3	1:A:15:ARG:H	1.41	0.85
1:E:145:VAL:HG13	1:E:146:GLU:N	1.88	0.85
1:C:143:TYR:CD1	1:C:144:PRO:HD3	2.11	0.85
1:E:143:TYR:CB	1:E:144:PRO:HD3	2.06	0.85
1:F:145:VAL:O	1:F:146:GLU:HB3	1.77	0.84
1:F:142:ASN:CB	1:F:148:PHE:HD2	1.88	0.84
1:A:201:ILE:HD13	1:A:210:ARG:HH12	1.42	0.83
1:C:117:ASN:O	1:D:173:LYS:HD2	1.79	0.82
1:F:226:GLN:O	1:F:228:GLN:CG	2.27	0.82
1:C:65:GLU:HA	1:C:68:ASP:HB2	1.63	0.81
1:B:142:ASN:HB3	1:B:144:PRO:HD2	1.63	0.81
1:A:7:TRP:O	1:A:10:LEU:O	1.99	0.81
1:D:139:LEU:HD12	1:D:153:VAL:HG21	1.62	0.80
1:F:63:LEU:HG	1:F:120:GLN:HE22	1.46	0.80
1:E:187:ALA:HB3	1:E:210:ARG:HH12	1.46	0.79
1:F:143:TYR:CD1	1:F:145:VAL:HG21	2.07	0.79
1:A:58:GLU:CG	1:A:59:ILE:N	2.45	0.79
2:D:301:PEE:C10	2:D:301:PEE:O3	2.31	0.79
1:F:200:PRO:HB3	1:F:206:LYS:NZ	1.98	0.79
1:D:11:GLU:O	1:D:15:ARG:HG2	1.82	0.78
1:E:144:PRO:O	1:E:145:VAL:HB	1.81	0.78
1:F:145:VAL:CG1	1:F:145:VAL:O	2.31	0.78
1:F:144:PRO:HB3	1:F:145:VAL:C	2.04	0.78
1:F:150:THR:O	1:F:151:LEU:HD12	1.83	0.78
1:E:142:ASN:N	1:E:142:ASN:ND2	2.30	0.78
1:A:204:ALA:HB1	1:A:206:LYS:HD3	1.66	0.77
1:C:171:LEU:O	1:C:174:GLN:N	2.18	0.77
1:F:144:PRO:HB2	1:F:147:LYS:N	2.00	0.77
1:D:261:TRP:CD1	1:D:261:TRP:C	2.57	0.77
1:E:145:VAL:HG13	1:E:146:GLU:CD	2.06	0.77
1:F:67:TYR:CE1	1:F:171:LEU:HD12	2.20	0.77
1:B:143:TYR:N	1:B:144:PRO:CD	2.49	0.76
1:F:35:SER:HB3	1:F:143:TYR:HE1	1.51	0.75
1:E:171:LEU:O	1:E:174:GLN:N	2.20	0.75
1:A:57:LYS:O	1:A:58:GLU:HB3	1.85	0.75
1:B:141:LEU:HD11	1:B:233:VAL:HG22	1.69	0.75
1:D:12:SER:HB3	1:D:15:ARG:CZ	2.17	0.75
1:F:226:GLN:C	1:F:228:GLN:N	2.24	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ASN:N	1:E:142:ASN:HD22	1.85	0.74
1:B:205:THR:HG23	1:B:206:LYS:HG3	1.69	0.74
1:C:200:PRO:HB2	1:C:210:ARG:HH21	1.51	0.73
1:B:142:ASN:C	1:B:144:PRO:HD2	2.09	0.72
1:F:150:THR:O	1:F:151:LEU:CD1	2.38	0.72
1:E:145:VAL:HG12	1:E:146:GLU:N	2.02	0.72
1:E:170:CYS:HB3	1:E:175:LEU:HD23	1.71	0.72
1:B:143:TYR:CD1	1:B:143:TYR:N	2.56	0.72
1:A:58:GLU:CG	1:A:59:ILE:H	2.03	0.72
1:A:12:SER:O	1:A:16:LEU:HB3	1.89	0.71
1:F:143:TYR:HA	1:F:144:PRO:C	2.10	0.71
1:F:12:SER:HB3	1:F:14:ASN:HB2	1.72	0.71
1:A:10:LEU:HD23	1:A:11:GLU:N	2.04	0.71
1:B:141:LEU:HB3	1:B:142:ASN:HD22	1.56	0.71
1:F:22:LYS:HA	1:F:25:ASN:HB2	1.73	0.70
1:F:68:ASP:HA	1:F:71:ARG:HG2	1.72	0.70
1:D:41:ARG:HG3	1:D:41:ARG:HH11	1.55	0.70
1:E:141:LEU:HD23	1:E:143:TYR:OH	1.91	0.69
1:E:145:VAL:HG13	1:E:146:GLU:OE1	1.92	0.69
1:F:140:VAL:CG2	1:F:145:VAL:N	2.28	0.69
1:A:143:TYR:CB	1:A:144:PRO:CD	2.71	0.69
1:A:146:GLU:O	1:A:148:PHE:N	2.26	0.68
1:E:142:ASN:ND2	1:E:142:ASN:H	1.86	0.68
1:F:144:PRO:CB	1:F:145:VAL:C	2.62	0.68
1:F:224:GLY:O	1:F:227:TYR:CE2	2.45	0.68
1:D:262:ILE:HD13	2:D:301:PEE:H13	1.74	0.68
1:F:147:LYS:O	1:F:148:PHE:HB2	1.94	0.68
1:D:22:LYS:HA	1:D:25:ASN:HB2	1.75	0.67
1:C:173:LYS:HG2	1:D:117:ASN:HB3	1.76	0.67
1:E:117:ASN:ND2	1:F:117:ASN:OD1	2.27	0.67
1:D:38:SER:OG	1:D:138:ASP:HB2	1.93	0.67
1:E:187:ALA:HB3	1:E:210:ARG:NH1	2.10	0.66
1:E:212:SER:OG	1:E:214:VAL:O	2.13	0.65
1:C:143:TYR:N	1:C:143:TYR:CD2	2.64	0.64
1:B:43:LEU:HD11	1:B:136:GLY:HA3	1.78	0.64
1:A:171:LEU:O	1:A:174:GLN:N	2.31	0.64
1:A:201:ILE:HD13	1:A:210:ARG:NH1	2.10	0.64
1:B:142:ASN:HB3	1:B:144:PRO:CD	2.28	0.64
1:F:35:SER:HB3	1:F:143:TYR:CE1	2.32	0.64
1:A:173:LYS:HE3	1:A:267:ASN:OD1	1.98	0.64
1:D:12:SER:OG	1:D:13:ASP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:HB3	1:A:209:GLU:CD	2.18	0.64
1:A:172:SER:HB3	1:B:117:ASN:HA	1.79	0.64
1:F:249:LYS:O	1:F:253:ARG:NH1	2.31	0.63
1:A:143:TYR:HB2	1:A:144:PRO:CD	2.26	0.63
1:A:209:GLU:OE1	1:A:209:GLU:N	2.32	0.63
1:A:9:THR:HG21	1:B:57:LYS:HA	1.81	0.63
1:D:172:SER:N	1:D:173:LYS:HA	2.14	0.63
1:D:261:TRP:HD1	1:D:261:TRP:C	2.00	0.63
1:A:143:TYR:CG	1:A:144:PRO:CD	2.78	0.63
1:A:27:TYR:OH	1:A:250:ASP:OD2	2.15	0.62
1:A:143:TYR:CB	1:A:144:PRO:HD3	2.27	0.62
1:F:226:GLN:O	1:F:227:TYR:C	2.37	0.62
1:D:200:PRO:HB2	1:D:210:ARG:NH2	2.15	0.62
1:D:12:SER:HB3	1:D:15:ARG:NH2	2.15	0.62
1:F:155:LEU:HG	1:F:221:THR:HG22	1.82	0.61
1:F:142:ASN:CB	1:F:148:PHE:CD2	2.72	0.61
1:F:149:MET:C	1:F:150:THR:HG23	2.20	0.61
1:F:226:GLN:C	1:F:228:GLN:HG2	2.21	0.61
1:F:147:LYS:O	1:F:148:PHE:CB	2.48	0.61
1:C:143:TYR:CG	1:C:144:PRO:HD3	2.35	0.61
1:F:169:ALA:HB3	1:F:176:PHE:HB2	1.82	0.61
1:B:67:TYR:HE1	1:B:171:LEU:HD21	1.65	0.61
1:E:176:PHE:CD1	1:E:263:ASN:HB2	2.36	0.61
1:B:249:LYS:HE2	1:B:253:ARG:NH2	2.15	0.60
1:B:249:LYS:HE2	1:B:253:ARG:HH22	1.66	0.60
1:D:153:VAL:HG22	1:D:223:ILE:HG22	1.83	0.60
1:D:261:TRP:HD1	1:D:261:TRP:O	1.85	0.60
1:F:155:LEU:HD22	1:F:244:LEU:HD22	1.83	0.59
1:F:190:ASP:HB2	1:F:192:GLN:HG3	1.84	0.59
1:C:139:LEU:HD12	1:C:153:VAL:HG21	1.84	0.59
1:F:140:VAL:HG21	1:F:145:VAL:CA	2.31	0.59
1:A:10:LEU:C	1:A:10:LEU:HD23	2.21	0.59
1:F:144:PRO:CA	1:F:145:VAL:CB	2.67	0.59
1:F:173:LYS:HD2	1:F:173:LYS:O	2.03	0.59
1:B:142:ASN:HB2	1:B:148:PHE:HB3	1.84	0.58
1:E:176:PHE:HD1	1:E:263:ASN:HB2	1.68	0.58
1:B:142:ASN:CB	1:B:144:PRO:HD2	2.33	0.58
1:D:14:ASN:C	1:D:14:ASN:OD1	2.42	0.58
1:D:66:PHE:O	1:D:70:ILE:HG12	2.03	0.58
1:A:206:LYS:HB3	1:A:209:GLU:OE1	2.04	0.58
1:B:139:LEU:HD13	1:B:240:LEU:HD22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:LEU:HD21	1:E:179:PHE:HE2	1.68	0.58
1:A:58:GLU:HG2	1:A:59:ILE:N	2.19	0.57
1:C:117:ASN:ND2	1:D:173:LYS:HE2	2.18	0.57
1:E:153:VAL:HG22	1:E:223:ILE:HG22	1.86	0.57
1:E:22:LYS:HG3	1:E:23:HIS:N	2.19	0.57
1:F:153:VAL:HG22	1:F:223:ILE:HG22	1.86	0.57
1:D:151:LEU:HD11	1:D:227:TYR:CE2	2.40	0.57
1:D:212:SER:HA	1:D:253:ARG:HH22	1.69	0.56
1:D:143:TYR:CD1	1:D:144:PRO:HD2	2.39	0.56
1:D:262:ILE:CD1	2:D:301:PEE:H13	2.36	0.56
1:A:153:VAL:HG22	1:A:223:ILE:HG22	1.87	0.56
1:B:188:LEU:HD21	1:B:201:ILE:HD11	1.88	0.56
1:D:65:GLU:HA	1:D:68:ASP:HB2	1.87	0.56
1:F:145:VAL:O	1:F:146:GLU:CB	2.49	0.56
1:F:176:PHE:HD1	1:F:263:ASN:HB2	1.71	0.56
1:C:174:GLN:NE2	1:C:267:ASN:ND2	2.30	0.56
1:C:61:ASP:N	1:C:61:ASP:OD1	2.38	0.56
1:D:210:ARG:N	1:D:210:ARG:HD3	2.18	0.56
1:D:115:SER:N	1:D:118:ASP:OD1	2.39	0.55
1:F:21:ARG:NH2	1:F:43:LEU:O	2.39	0.55
1:B:142:ASN:HB3	1:B:144:PRO:CG	2.35	0.55
1:B:56:LEU:HD11	1:B:59:ILE:HG13	1.87	0.55
1:E:244:LEU:HD12	1:E:247:ILE:HD11	1.87	0.55
1:F:115:SER:N	1:F:117:ASN:OD1	2.39	0.55
1:F:148:PHE:N	1:F:148:PHE:CD1	2.74	0.55
1:C:162:LEU:HD21	1:C:179:PHE:HE2	1.72	0.55
1:C:22:LYS:HZ2	1:C:41:ARG:HH12	1.54	0.55
1:A:70:ILE:HA	1:A:72:GLU:OE1	2.06	0.55
1:B:141:LEU:O	1:B:141:LEU:HD12	2.07	0.55
1:B:142:ASN:HB3	1:B:144:PRO:HG2	1.88	0.55
1:B:257:ALA:O	1:B:260:SER:N	2.39	0.55
1:D:67:TYR:HE1	1:D:171:LEU:HD13	1.72	0.55
1:B:141:LEU:HB3	1:B:142:ASN:ND2	2.21	0.55
1:F:226:GLN:O	1:F:228:GLN:CA	2.50	0.55
1:A:10:LEU:CD2	1:A:10:LEU:C	2.75	0.54
1:D:239:GLU:OE2	1:E:253:ARG:NH2	2.39	0.54
1:F:21:ARG:HG2	1:F:22:LYS:HG2	1.89	0.54
1:E:146:GLU:CD	1:E:146:GLU:H	2.11	0.54
1:C:21:ARG:HH12	1:C:22:LYS:HZ2	1.56	0.54
1:F:12:SER:HB2	1:F:15:ARG:H	1.73	0.54
1:C:185:ASP:OD1	1:C:210:ARG:NH1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:TYR:O	1:D:71:ARG:HG3	2.08	0.54
1:B:142:ASN:CG	1:B:148:PHE:HD2	2.11	0.54
1:F:224:GLY:O	1:F:225:GLU:CB	2.56	0.54
1:D:162:LEU:HD21	1:D:179:PHE:HE2	1.74	0.53
1:D:169:ALA:O	1:D:176:PHE:N	2.39	0.53
1:D:171:LEU:C	1:D:173:LYS:HA	2.28	0.53
1:B:208:LEU:HD21	1:C:245:PHE:CG	2.42	0.53
1:C:249:LYS:HA	1:C:252:LEU:HD12	1.91	0.53
1:A:62:PRO:HA	1:A:120:GLN:NE2	2.13	0.53
1:F:146:GLU:O	1:F:146:GLU:HG3	2.09	0.52
1:E:67:TYR:O	1:E:70:ILE:HG13	2.09	0.52
1:B:60:THR:OG1	1:B:61:ASP:N	2.42	0.52
1:C:117:ASN:HB2	1:D:173:LYS:HG3	1.91	0.52
1:C:189:ASP:O	1:C:190:ASP:HB3	2.10	0.52
1:E:121:PHE:HB2	1:E:123:LEU:HD11	1.92	0.52
1:F:206:LYS:HG3	1:F:206:LYS:O	2.10	0.52
1:F:213:ILE:HD12	1:F:214:VAL:HG23	1.91	0.52
1:C:187:ALA:HB3	1:C:210:ARG:NH1	2.25	0.52
1:E:172:SER:O	1:E:172:SER:OG	2.27	0.52
1:A:181:CYS:SG	1:A:210:ARG:NH2	2.83	0.52
1:B:141:LEU:HB2	1:B:149:MET:O	2.10	0.52
1:C:22:LYS:HA	1:C:25:ASN:HB2	1.91	0.52
1:C:265:ASP:OD2	1:C:267:ASN:ND2	2.43	0.52
1:B:23:HIS:O	1:B:26:SER:HB3	2.10	0.51
1:F:171:LEU:HD23	1:F:172:SER:N	2.25	0.51
1:A:189:ASP:O	1:A:190:ASP:HB3	2.10	0.51
1:A:57:LYS:HD3	1:A:124:GLU:HB2	1.93	0.51
1:C:22:LYS:NZ	1:C:41:ARG:HH12	2.08	0.51
1:A:12:SER:HB3	1:A:15:ARG:N	2.19	0.51
1:A:120:GLN:OE1	1:A:167:ILE:HB	2.10	0.51
1:C:251:PHE:CE1	1:C:255:GLU:HG3	2.46	0.51
1:F:148:PHE:HD1	1:F:148:PHE:N	2.09	0.51
1:C:164:SER:HB2	1:C:181:CYS:O	2.11	0.50
1:C:196:ASP:OD1	1:C:198:LYS:HB2	2.11	0.50
1:F:149:MET:O	1:F:150:THR:HG23	2.11	0.50
1:B:239:GLU:HG3	1:B:239:GLU:O	2.12	0.50
1:F:151:LEU:HD11	1:F:227:TYR:CZ	2.47	0.50
1:F:181:CYS:SG	1:F:182:ASP:N	2.84	0.50
1:A:146:GLU:O	1:A:147:LYS:C	2.50	0.50
1:A:20:ILE:HG23	2:A:301:PEE:H48	1.92	0.50
1:C:66:PHE:O	1:C:69:SER:OG	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LEU:CD1	1:B:153:VAL:HB	2.42	0.49
1:A:145:VAL:HG12	1:A:146:GLU:N	2.27	0.49
1:F:224:GLY:C	1:F:225:GLU:HG3	2.33	0.49
1:A:208:LEU:N	1:A:209:GLU:OE1	2.44	0.49
1:F:159:ASP:OD2	1:F:218:LYS:HD2	2.13	0.49
1:A:12:SER:HB2	1:A:15:ARG:HD2	1.95	0.49
1:D:181:CYS:SG	1:D:182:ASP:N	2.85	0.49
1:A:12:SER:CB	1:A:15:ARG:HB2	2.43	0.49
1:A:12:SER:HB3	1:A:15:ARG:HB2	1.93	0.49
1:A:70:ILE:HD12	1:A:171:LEU:HD12	1.94	0.49
1:B:162:LEU:HD21	1:B:179:PHE:HE2	1.78	0.49
1:C:66:PHE:CD1	1:C:176:PHE:HD2	2.30	0.49
1:E:162:LEU:HD21	1:E:179:PHE:CE2	2.48	0.49
1:C:153:VAL:HG22	1:C:223:ILE:HG22	1.95	0.49
1:A:28:LEU:O	1:A:31:THR:HG22	2.13	0.48
1:E:55:THR:HG23	1:F:6:ASN:HB3	1.94	0.48
1:D:11:GLU:HG2	1:D:16:LEU:HB2	1.95	0.48
1:D:201:ILE:HD13	1:D:210:ARG:NH1	2.28	0.48
1:F:12:SER:CB	1:F:14:ASN:HB2	2.40	0.48
1:B:167:ILE:HG12	1:B:180:LEU:HD13	1.94	0.48
1:B:237:VAL:O	1:B:241:GLU:HG3	2.13	0.48
1:E:61:ASP:N	1:E:61:ASP:OD1	2.34	0.48
1:B:58:GLU:HB2	1:B:122:LEU:HD23	1.95	0.48
1:C:70:ILE:O	1:C:70:ILE:HG22	2.14	0.48
1:C:232:SER:O	1:C:235:ARG:HG2	2.14	0.47
1:D:127:TYR:HB3	1:D:162:LEU:HB3	1.96	0.47
1:D:262:ILE:HD11	2:D:301:PEE:C30	2.44	0.47
1:F:263:ASN:O	1:F:264:LEU:HD23	2.14	0.47
1:A:177:LEU:HB3	1:A:262:ILE:HD11	1.95	0.47
1:D:13:ASP:O	1:D:14:ASN:CB	2.61	0.47
1:B:142:ASN:CA	1:B:144:PRO:HD2	2.44	0.47
1:D:262:ILE:HG21	2:D:301:PEE:O4	2.15	0.47
1:F:127:TYR:HB3	1:F:162:LEU:HB3	1.97	0.47
1:F:224:GLY:O	1:F:225:GLU:HB2	2.15	0.47
1:A:12:SER:O	1:A:16:LEU:CB	2.59	0.47
1:D:262:ILE:HD13	2:D:301:PEE:C11	2.44	0.47
1:C:181:CYS:SG	1:C:182:ASP:N	2.88	0.47
1:A:9:THR:HG21	1:B:57:LYS:O	2.15	0.47
1:F:36:TYR:HA	1:F:140:VAL:HG12	1.96	0.47
1:C:187:ALA:HB3	1:C:210:ARG:NH2	2.30	0.47
1:E:176:PHE:HE1	1:E:263:ASN:HD22	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:SER:HA	1:A:173:LYS:HA	1.57	0.46
1:B:145:VAL:HG12	1:B:146:GLU:H	1.79	0.46
1:E:118:ASP:HB3	1:E:171:LEU:HG	1.97	0.46
1:B:39:ASN:O	1:B:137:ALA:HA	2.15	0.46
1:D:213:ILE:H	1:D:253:ARG:NH2	2.13	0.46
1:B:54:ILE:CG2	1:B:123:LEU:HD23	2.45	0.46
1:B:163:HIS:ND1	1:B:183:VAL:HG21	2.30	0.46
1:B:28:LEU:O	1:B:31:THR:HG22	2.16	0.46
1:A:265:ASP:OD1	1:A:266:PHE:N	2.49	0.46
1:F:67:TYR:CZ	1:F:171:LEU:HD12	2.51	0.46
1:C:170:CYS:HB3	1:C:175:LEU:HD23	1.98	0.46
1:F:165:LEU:HD13	1:F:194:VAL:HG21	1.98	0.46
1:F:67:TYR:HB3	1:F:71:ARG:HH12	1.80	0.46
1:A:121:PHE:HB3	1:A:123:LEU:HD21	1.97	0.46
1:C:265:ASP:OD1	1:C:266:PHE:N	2.48	0.46
1:D:12:SER:CB	1:D:15:ARG:NH2	2.79	0.46
1:B:135:ILE:HD13	1:B:244:LEU:HD11	1.99	0.45
1:C:163:HIS:HD2	1:C:183:VAL:HB	1.80	0.45
1:E:142:ASN:O	1:E:143:TYR:CD1	2.70	0.45
1:A:11:GLU:CG	1:A:12:SER:HB2	2.45	0.45
1:B:180:LEU:HD11	1:B:258:TRP:CE3	2.51	0.45
1:D:41:ARG:HG3	1:D:41:ARG:NH1	2.26	0.45
1:F:194:VAL:HG13	1:F:201:ILE:HD12	1.99	0.45
1:D:61:ASP:OD1	1:D:61:ASP:N	2.46	0.45
1:A:66:PHE:HB3	1:A:171:LEU:HD11	1.99	0.45
1:A:70:ILE:CA	1:A:72:GLU:HB3	2.46	0.45
1:D:164:SER:HB2	1:D:181:CYS:O	2.17	0.45
1:D:168:VAL:HA	1:D:176:PHE:O	2.17	0.45
2:D:301:PEE:C1	2:D:301:PEE:O4	2.63	0.45
1:A:68:ASP:C	1:A:70:ILE:H	2.20	0.45
1:C:143:TYR:CZ	1:C:147:LYS:HG2	2.51	0.45
1:B:208:LEU:HD12	1:C:241:GLU:HB3	1.99	0.45
1:D:13:ASP:O	1:D:14:ASN:CG	2.55	0.45
1:D:262:ILE:CG2	2:D:301:PEE:O4	2.64	0.45
1:A:59:ILE:O	1:A:60:THR:CG2	2.65	0.45
1:E:231:GLY:HA2	1:E:234:LEU:HD12	1.99	0.45
1:E:66:PHE:CE1	1:E:176:PHE:HD2	2.34	0.45
1:B:225:GLU:OE1	1:B:225:GLU:N	2.43	0.44
1:C:194:VAL:C	1:C:196:ASP:H	2.19	0.44
1:E:163:HIS:ND1	1:E:183:VAL:HG21	2.32	0.44
1:B:208:LEU:HD21	1:C:245:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:HG12	1:A:146:GLU:H	1.83	0.44
1:A:209:GLU:O	1:A:210:ARG:HD2	2.18	0.44
1:A:245:PHE:CE1	1:A:249:LYS:HE3	2.53	0.44
2:A:301:PEE:H2	2:A:301:PEE:O4	2.17	0.44
1:A:9:THR:CG2	1:B:57:LYS:HA	2.46	0.44
1:B:142:ASN:ND2	1:B:148:PHE:HD2	2.16	0.44
1:E:127:TYR:HB3	1:E:162:LEU:HB3	2.00	0.44
1:E:6:ASN:HB3	1:F:55:THR:HG23	2.00	0.44
1:F:226:GLN:CA	1:F:228:GLN:HG2	2.48	0.44
1:A:127:TYR:HB3	1:A:162:LEU:HB3	1.99	0.43
1:B:121:PHE:HB2	1:B:123:LEU:HD11	2.00	0.43
1:F:144:PRO:CA	1:F:145:VAL:C	2.86	0.43
1:B:165:LEU:HD13	1:B:194:VAL:HG21	2.00	0.43
1:C:187:ALA:HB3	1:C:210:ARG:HH12	1.82	0.43
1:A:9:THR:HG21	1:B:57:LYS:CA	2.45	0.43
1:B:142:ASN:ND2	1:B:148:PHE:CD2	2.86	0.43
1:B:155:LEU:HD22	1:B:244:LEU:HD22	2.00	0.43
1:D:144:PRO:C	1:D:146:GLU:N	2.72	0.43
1:D:162:LEU:HD21	1:D:179:PHE:CE2	2.53	0.43
1:E:117:ASN:HB3	1:F:172:SER:OG	2.18	0.43
1:C:173:LYS:HD2	1:C:173:LYS:HA	1.70	0.43
1:F:141:LEU:HD11	1:F:149:MET:HB2	2.01	0.43
1:B:177:LEU:HD12	1:B:178:SER:H	1.83	0.43
1:F:147:LYS:HG2	1:F:148:PHE:CD1	2.54	0.43
1:A:12:SER:CB	1:A:15:ARG:HD2	2.49	0.43
1:A:151:LEU:HD11	1:A:227:TYR:CZ	2.54	0.43
1:A:70:ILE:CD1	1:A:171:LEU:HD12	2.48	0.43
1:B:123:LEU:N	1:B:123:LEU:HD12	2.34	0.43
1:D:121:PHE:HB3	1:D:123:LEU:HD21	2.01	0.43
1:A:189:ASP:C	1:A:191:ASN:H	2.21	0.43
1:B:22:LYS:HD2	1:B:22:LYS:HA	1.76	0.43
1:C:68:ASP:C	1:C:71:ARG:HB2	2.39	0.43
1:E:118:ASP:HB3	1:E:170:CYS:O	2.19	0.43
1:B:54:ILE:HG21	1:B:123:LEU:HD23	2.01	0.43
1:B:198:LYS:HD2	1:B:198:LYS:O	2.18	0.42
1:C:173:LYS:HG2	1:D:117:ASN:CB	2.47	0.42
1:B:249:LYS:O	1:B:252:LEU:HG	2.19	0.42
1:C:226:GLN:H	1:C:226:GLN:CD	2.23	0.42
1:D:144:PRO:C	1:D:146:GLU:H	2.22	0.42
1:D:27:TYR:O	1:D:31:THR:HG23	2.20	0.42
1:E:165:LEU:HD13	1:E:194:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:GLY:O	1:F:225:GLU:HG3	2.20	0.42
1:B:139:LEU:HB3	1:B:151:LEU:HG	2.01	0.42
1:D:226:GLN:HG3	1:D:226:GLN:H	1.45	0.42
1:F:164:SER:HB2	1:F:181:CYS:O	2.20	0.42
1:D:261:TRP:CD1	1:D:261:TRP:O	2.68	0.42
1:E:145:VAL:CG1	1:E:146:GLU:OE1	2.64	0.42
2:A:301:PEE:O4	2:A:301:PEE:C1	2.67	0.42
1:D:253:ARG:N	1:D:253:ARG:HD2	2.35	0.42
1:E:185:ASP:OD1	1:E:210:ARG:CZ	2.68	0.42
1:B:151:LEU:HD12	1:B:151:LEU:O	2.19	0.42
1:E:155:LEU:HD22	1:E:244:LEU:HD22	2.01	0.42
1:F:253:ARG:HD3	1:F:253:ARG:HA	1.90	0.42
1:A:13:ASP:O	1:A:17:ASN:ND2	2.53	0.41
1:C:174:GLN:OE1	1:C:174:GLN:HA	2.19	0.41
1:C:165:LEU:HD13	1:C:194:VAL:HG21	2.02	0.41
2:A:301:PEE:O3	2:A:301:PEE:C10	2.68	0.41
1:B:33:LEU:HA	1:B:34:PRO:HD3	1.85	0.41
1:C:21:ARG:HH12	1:C:22:LYS:NZ	2.18	0.41
1:D:143:TYR:CG	1:D:144:PRO:HD2	2.55	0.41
1:E:139:LEU:HD13	1:E:240:LEU:HD22	2.03	0.41
1:A:11:GLU:HG2	1:A:15:ARG:HD2	2.02	0.41
1:D:116:PRO:HA	1:D:117:ASN:HA	1.73	0.41
1:D:11:GLU:O	1:D:12:SER:HB3	2.20	0.41
1:E:262:ILE:HD13	1:E:262:ILE:HA	1.83	0.41
1:A:116:PRO:HA	1:A:117:ASN:HA	1.54	0.41
1:B:161:GLY:HA3	1:B:216:SER:HB3	2.03	0.41
1:E:57:LYS:HA	1:E:57:LYS:HD2	1.91	0.41
1:F:150:THR:O	1:F:151:LEU:HD13	2.17	0.41
1:F:176:PHE:CD1	1:F:263:ASN:HB2	2.52	0.41
1:A:256:LEU:HD11	2:A:301:PEE:H50	2.01	0.41
1:A:70:ILE:HA	1:A:72:GLU:HB3	2.03	0.41
1:C:242:GLN:O	1:C:245:PHE:HB3	2.21	0.41
1:C:155:LEU:HD22	1:C:244:LEU:HD22	2.02	0.41
1:E:173:LYS:HB3	1:E:265:ASP:OD2	2.20	0.41
1:C:168:VAL:HG22	1:C:177:LEU:HD13	2.03	0.41
1:F:45:PHE:CE2	1:F:131:LEU:HD21	2.56	0.41
1:A:245:PHE:O	1:A:249:LYS:HG3	2.21	0.41
1:A:59:ILE:O	1:A:60:THR:HG23	2.20	0.41
1:D:228:GLN:HG3	1:D:228:GLN:H	1.69	0.41
1:E:135:ILE:HD13	1:E:244:LEU:HD11	2.03	0.41
1:E:181:CYS:SG	1:E:182:ASP:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:ILE:HG13	1:F:253:ARG:CZ	2.51	0.41
1:B:194:VAL:HG13	1:B:201:ILE:HD12	2.03	0.41
1:C:151:LEU:HD11	1:C:227:TYR:CD2	2.57	0.41
1:A:162:LEU:HD21	1:A:179:PHE:HE2	1.85	0.40
1:F:185:ASP:HA	1:F:186:PRO:HD3	1.89	0.40
1:F:173:LYS:HG3	1:F:265:ASP:OD2	2.21	0.40
1:F:67:TYR:O	1:F:71:ARG:HG2	2.21	0.40
1:A:162:LEU:HD21	1:A:179:PHE:CE2	2.56	0.40
1:A:242:GLN:O	1:A:245:PHE:HB3	2.21	0.40
1:C:258:TRP:CD2	1:C:259:PRO:HA	2.56	0.40
1:E:230:GLN:HB2	1:E:233:VAL:HG23	2.03	0.40
1:B:67:TYR:HE1	1:B:171:LEU:CD2	2.30	0.40
1:C:265:ASP:OD1	1:C:267:ASN:CG	2.60	0.40
1:A:12:SER:OG	1:A:15:ARG:NH1	2.52	0.40
1:A:256:LEU:HD21	2:A:301:PEE:H56	2.02	0.40
1:D:38:SER:HG	1:D:138:ASP:HB2	1.84	0.40
2:D:301:PEE:H14	2:D:301:PEE:H49	2.03	0.40
1:E:54:ILE:CG2	1:E:123:LEU:HD23	2.50	0.40
1:F:149:MET:O	1:F:150:THR:CB	2.69	0.40
1:F:12:SER:HB2	1:F:15:ARG:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	223/236 (94%)	199 (89%)	16 (7%)	8 (4%)	3 29
1	B	219/236 (93%)	208 (95%)	8 (4%)	3 (1%)	11 48
1	C	222/236 (94%)	210 (95%)	9 (4%)	3 (1%)	11 48
1	D	223/236 (94%)	206 (92%)	15 (7%)	2 (1%)	17 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	222/236 (94%)	210 (95%)	8 (4%)	4 (2%)	8	43
1	F	221/236 (94%)	199 (90%)	15 (7%)	7 (3%)	4	31
All	All	1330/1416 (94%)	1232 (93%)	71 (5%)	27 (2%)	7	41

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	GLU
1	A	147	LYS
1	C	71	ARG
1	C	172	SER
1	E	145	VAL
1	F	227	TYR
1	D	144	PRO
1	E	172	SER
1	A	201	ILE
1	B	116	PRO
1	E	143	TYR
1	E	144	PRO
1	F	142	ASN
1	F	146	GLU
1	F	148	PHE
1	F	189	ASP
1	A	145	VAL
1	A	204	ALA
1	B	145	VAL
1	D	145	VAL
1	F	12	SER
1	F	32	GLN
1	A	58	GLU
1	A	143	TYR
1	C	143	TYR
1	B	201	ILE
1	A	206	LYS

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	209/213 (98%)	195 (93%)	14 (7%)	16	50
1	B	205/213 (96%)	199 (97%)	6 (3%)	42	72
1	C	208/213 (98%)	203 (98%)	5 (2%)	49	75
1	D	209/213 (98%)	203 (97%)	6 (3%)	42	72
1	E	208/213 (98%)	199 (96%)	9 (4%)	29	63
1	F	207/213 (97%)	196 (95%)	11 (5%)	22	58
All	All	1246/1278 (98%)	1195 (96%)	51 (4%)	30	64

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	11	GLU
1	A	38	SER
1	A	56	LEU
1	A	57	LYS
1	A	120	GLN
1	A	142	ASN
1	A	143	TYR
1	A	146	GLU
1	A	171	LEU
1	A	173	LYS
1	A	201	ILE
1	A	213	ILE
1	A	218	LYS
1	B	35	SER
1	B	123	LEU
1	B	141	LEU
1	B	143	TYR
1	B	239	GLU
1	B	261	TRP
1	C	65	GLU
1	C	143	TYR
1	C	208	LEU
1	C	209	GLU
1	C	261	TRP
1	D	11	GLU
1	D	12	SER

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Mol	Chain	Res	Type
1	D	13	ASP
1	D	14	ASN
1	D	226	GLN
1	D	261	TRP
1	E	15	ARG
1	E	22	LYS
1	E	41	ARG
1	E	61	ASP
1	E	123	LEU
1	E	142	ASN
1	E	146	GLU
1	E	261	TRP
1	E	263	ASN
1	F	73	GLU
1	F	117	ASN
1	F	142	ASN
1	F	146	GLU
1	F	149	MET
1	F	151	LEU
1	F	174	GLN
1	F	190	ASP
1	F	222	GLU
1	F	234	LEU
1	F	261	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	B	142	ASN
1	C	267	ASN
1	E	117	ASN
1	E	142	ASN
1	E	263	ASN
1	F	120	GLN
1	F	228	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEE	D	301	-	30,30,50	0.70	0	33,35,55	0.76	0
2	PEE	A	301	-	30,30,50	0.70	0	33,35,55	0.76	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
2	PEE	D	301	-	-	12/34/34/54	-
2	PEE	A	301	-	-	19/34/34/54	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	PEE	C1-O3P-P-O4P
2	A	301	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
2	A	301	PEE	C1-O3P-P-O1P
2	A	301	PEE	C1-O3P-P-O2P
2	A	301	PEE	C1-O3P-P-O4P
2	D	301	PEE	O5-C30-O3-C3
2	D	301	PEE	C31-C30-O3-C3
2	D	301	PEE	C11-C10-O2-C2
2	A	301	PEE	C32-C33-C34-C35
2	A	301	PEE	C11-C12-C13-C14
2	D	301	PEE	O4-C10-O2-C2
2	D	301	PEE	O4P-C4-C5-N
2	A	301	PEE	C11-C10-O2-C2
2	A	301	PEE	O4-C10-O2-C2
2	A	301	PEE	C31-C32-C33-C34
2	A	301	PEE	O2-C2-C3-O3
2	A	301	PEE	C1-C2-C3-O3
2	A	301	PEE	C4-O4P-P-O3P
2	D	301	PEE	C32-C33-C34-C35
2	A	301	PEE	C13-C14-C15-C16
2	D	301	PEE	O3P-C1-C2-C3
2	D	301	PEE	O3P-C1-C2-O2
2	D	301	PEE	C3-C2-O2-C10
2	A	301	PEE	C3-C2-O2-C10
2	A	301	PEE	O3P-C1-C2-C3
2	A	301	PEE	O3P-C1-C2-O2
2	A	301	PEE	C2-C1-O3P-P
2	D	301	PEE	O2-C2-C3-O3
2	A	301	PEE	O3-C30-C31-C32
2	D	301	PEE	C1-C2-O2-C10
2	A	301	PEE	O5-C30-C31-C32

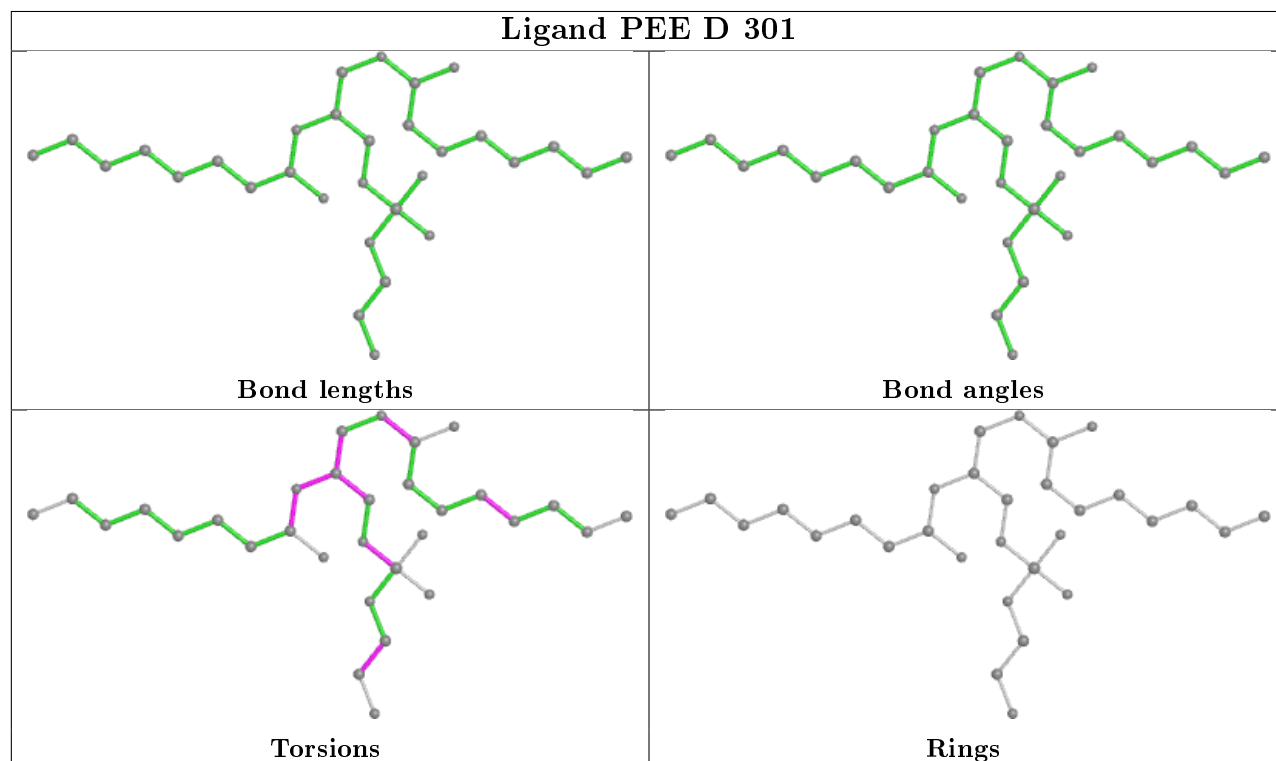
There are no ring outliers.

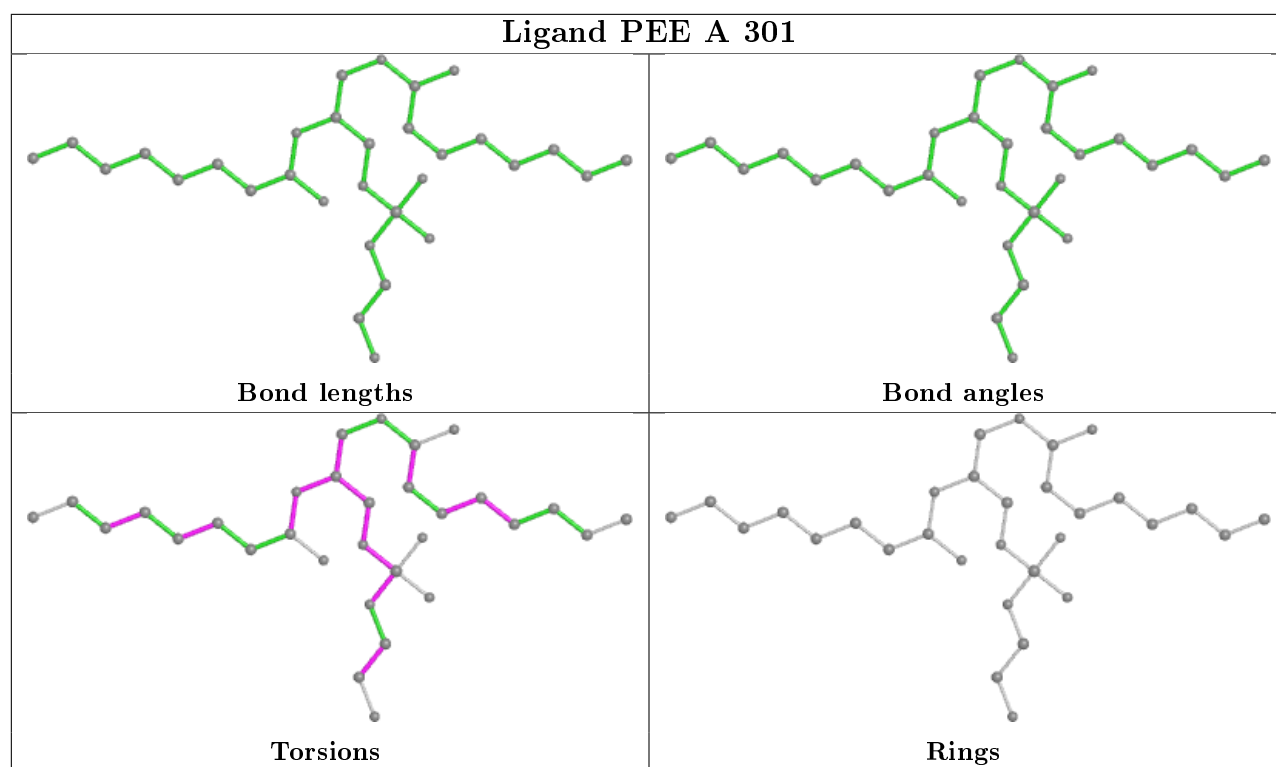
2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	PEE	9	0
2	A	301	PEE	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	227/236 (96%)	-0.32	4 (1%) 68 53	55, 95, 178, 264	0
1	B	223/236 (94%)	0.13	12 (5%) 25 16	62, 117, 187, 243	0
1	C	226/236 (95%)	-0.34	1 (0%) 92 86	54, 99, 179, 244	0
1	D	227/236 (96%)	-0.38	0 100 100	47, 92, 184, 223	0
1	E	226/236 (95%)	-0.22	5 (2%) 62 45	46, 93, 177, 257	0
1	F	225/236 (95%)	-0.07	4 (1%) 68 53	65, 111, 209, 259	0
All	All	1354/1416 (95%)	-0.20	26 (1%) 66 51	46, 101, 187, 264	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	73	GLU	5.0
1	B	228	GLN	3.8
1	B	141	LEU	3.6
1	B	143	TYR	3.4
1	E	146	GLU	3.1
1	F	145	VAL	3.0
1	B	142	ASN	3.0
1	F	72	GLU	2.9
1	E	72	GLU	2.8
1	B	145	VAL	2.7
1	E	144	PRO	2.6
1	E	143	TYR	2.6
1	E	73	GLU	2.5
1	B	63	LEU	2.5
1	C	72	GLU	2.5
1	B	223	ILE	2.4
1	A	144	PRO	2.3
1	A	71	ARG	2.3
1	A	145	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	143	TYR	2.2
1	B	190	ASP	2.2
1	F	228	GLN	2.2
1	B	191	ASN	2.1
1	B	115	SER	2.1
1	B	70	ILE	2.0
1	B	195	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

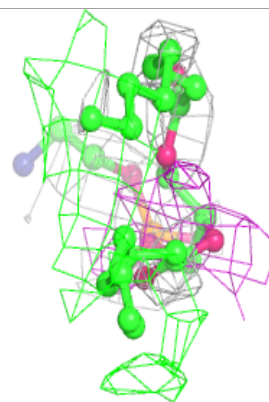
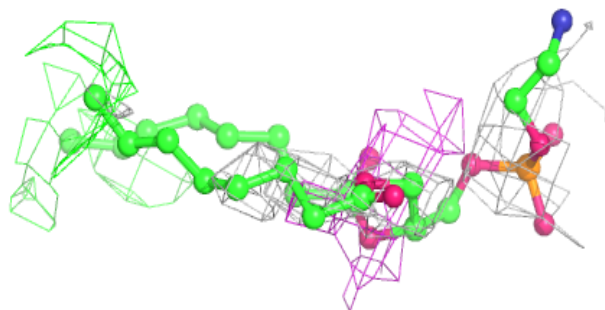
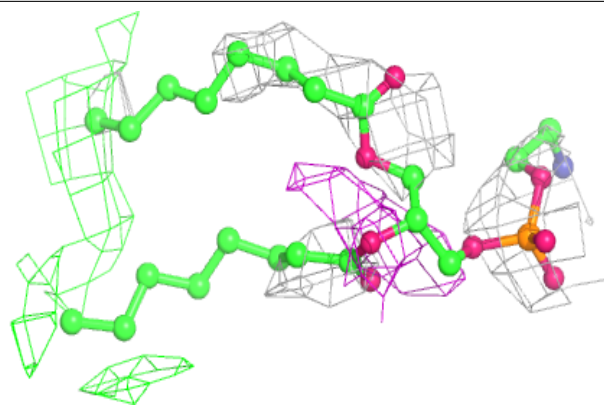
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEE	A	301	31/51	0.66	0.56	95,125,212,221	0
2	PEE	D	301	31/51	0.70	0.57	94,145,212,221	0

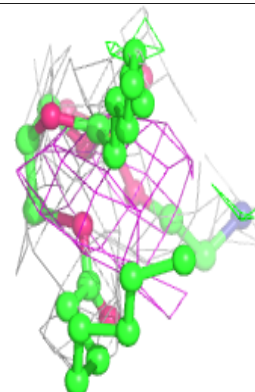
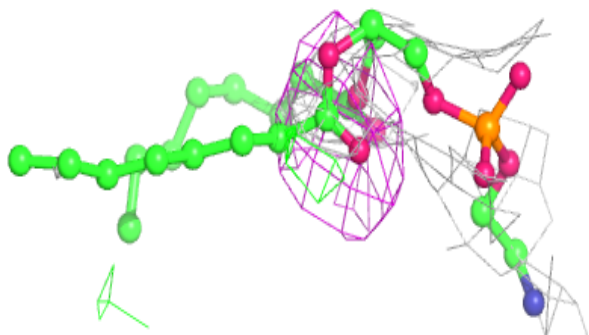
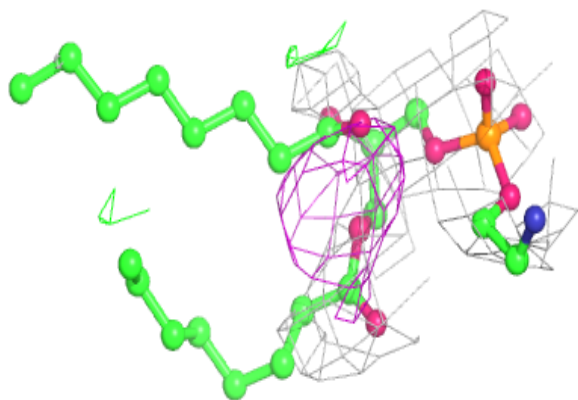
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEE A 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 D 301:**

$2mF_o-DF_c$ (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.