



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 12:25 PM BST

PDB ID : 5IZR
Title : Human GIVD cytosolic phospholipase A2 in complex with Methyl gamma-Linolenyl Fluorophosphonate inhibitor and Terbium Chloride
Authors : Wang, H.; Klein, M.G.
Deposited on : 2016-03-25
Resolution : 3.25 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 : 2.13
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) : 2.13

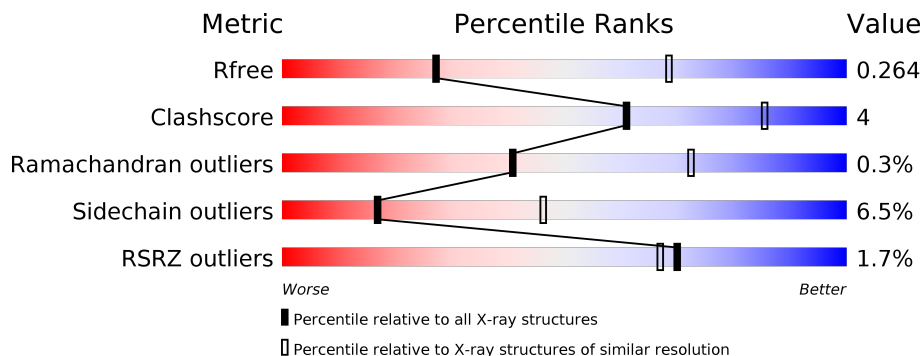
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	814	 % 69% 12% • 17%
1	B	814	 % 70% 12% • 17%
1	C	814	 % 68% 13% • 19%
1	D	814	 2% 69% 12% • 18%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 21369 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.

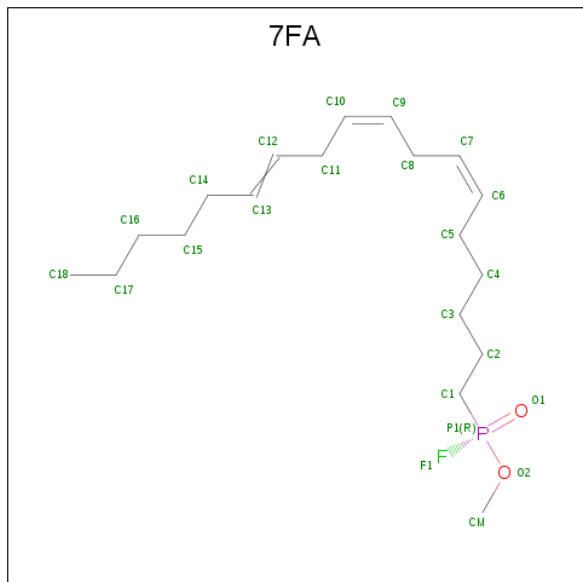
- Molecule 1 is a protein called Cytosolic phospholipase A2 delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	674	Total 5369	C 3426	N 915	O 1003	S 25	0	0	0
1	B	675	Total 5350	C 3415	N 902	O 1009	S 24	0	0	0
1	C	659	Total 5244	C 3344	N 889	O 987	S 24	0	0	0
1	D	664	Total 5291	C 3379	N 896	O 991	S 25	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q86XP0
A	-2	ALA	-	expression tag	UNP Q86XP0
A	-1	MET	-	expression tag	UNP Q86XP0
A	0	GLY	-	expression tag	UNP Q86XP0
A	1	SER	-	expression tag	UNP Q86XP0
B	-3	GLY	-	expression tag	UNP Q86XP0
B	-2	ALA	-	expression tag	UNP Q86XP0
B	-1	MET	-	expression tag	UNP Q86XP0
B	0	GLY	-	expression tag	UNP Q86XP0
B	1	SER	-	expression tag	UNP Q86XP0
C	-3	GLY	-	expression tag	UNP Q86XP0
C	-2	ALA	-	expression tag	UNP Q86XP0
C	-1	MET	-	expression tag	UNP Q86XP0
C	0	GLY	-	expression tag	UNP Q86XP0
C	1	SER	-	expression tag	UNP Q86XP0
D	-3	GLY	-	expression tag	UNP Q86XP0
D	-2	ALA	-	expression tag	UNP Q86XP0
D	-1	MET	-	expression tag	UNP Q86XP0
D	0	GLY	-	expression tag	UNP Q86XP0
D	1	SER	-	expression tag	UNP Q86XP0

- Molecule 2 is methyl (R)-(6Z,9Z,12Z)-octadeca-6,9,12-trien-1-ylphosphonofluoridate (three-letter code: 7FA) (formula: C₁₉H₃₄FO₂P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	22	19	2	1	0	0
2	B	1	22	19	2	1	0	0
2	C	1	22	19	2	1	0	0
2	D	1	22	19	2	1	0	0

- Molecule 3 is TERBIUM(III) ION (three-letter code: TB) (formula: Tb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Tb		
3	B	4	4	4	0	0
3	A	4	4	4	0	0
3	D	4	4	4	0	0
3	C	3	3	3	0	0

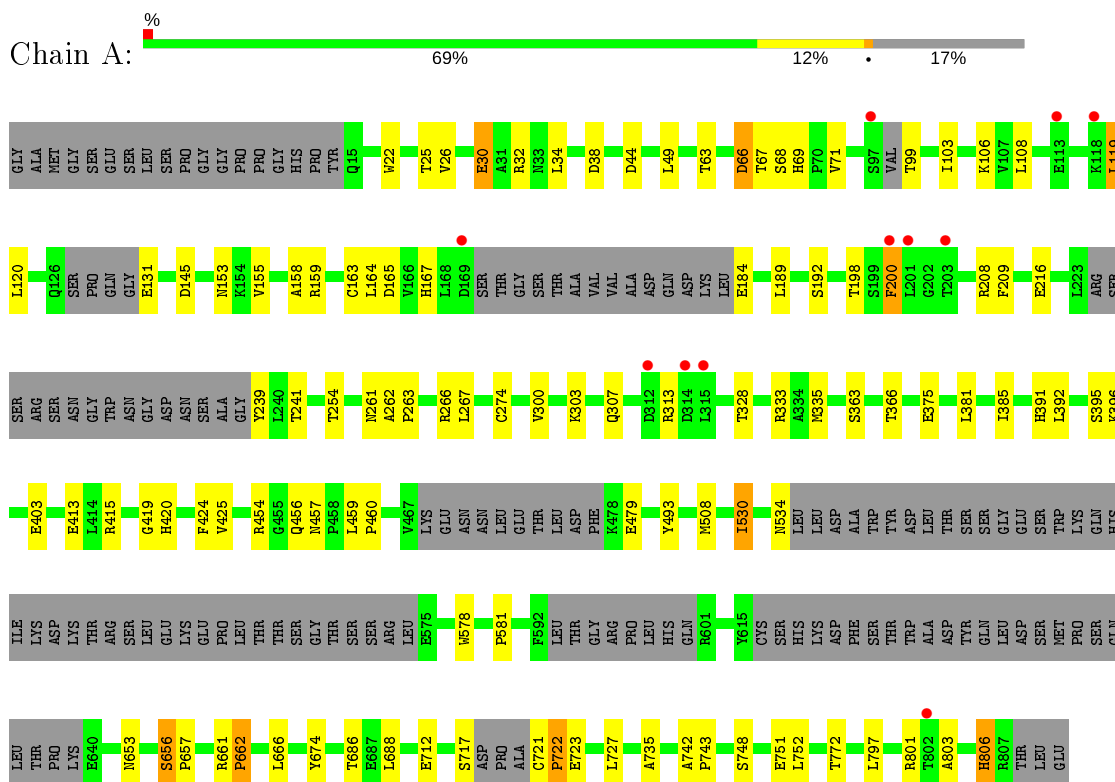
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	2	Total O 2 2	0	0
4	C	2	Total O 2 2	0	0
4	D	5	Total O 5 5	0	0

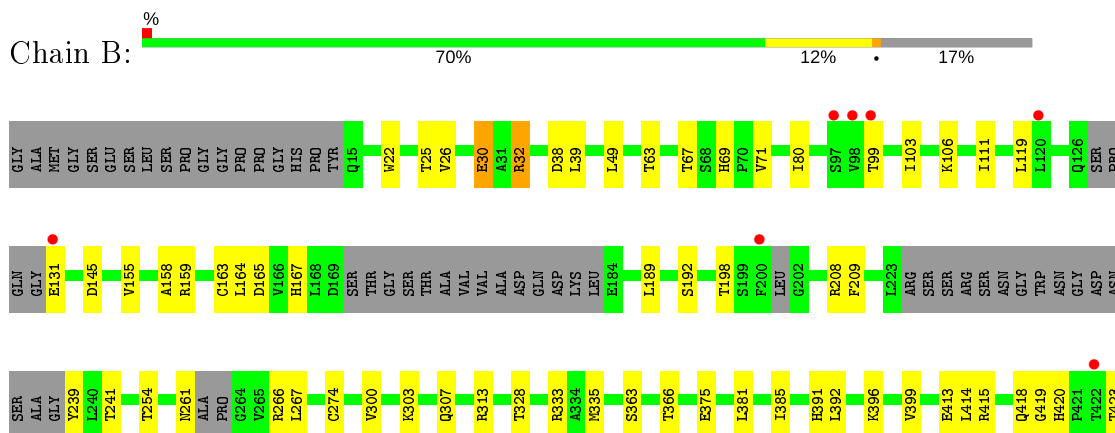
3 Residue-property plots

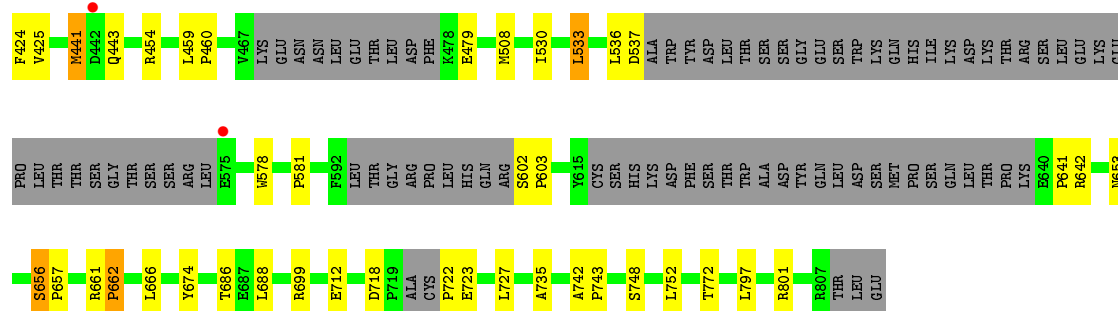
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cytosolic phospholipase A2 delta

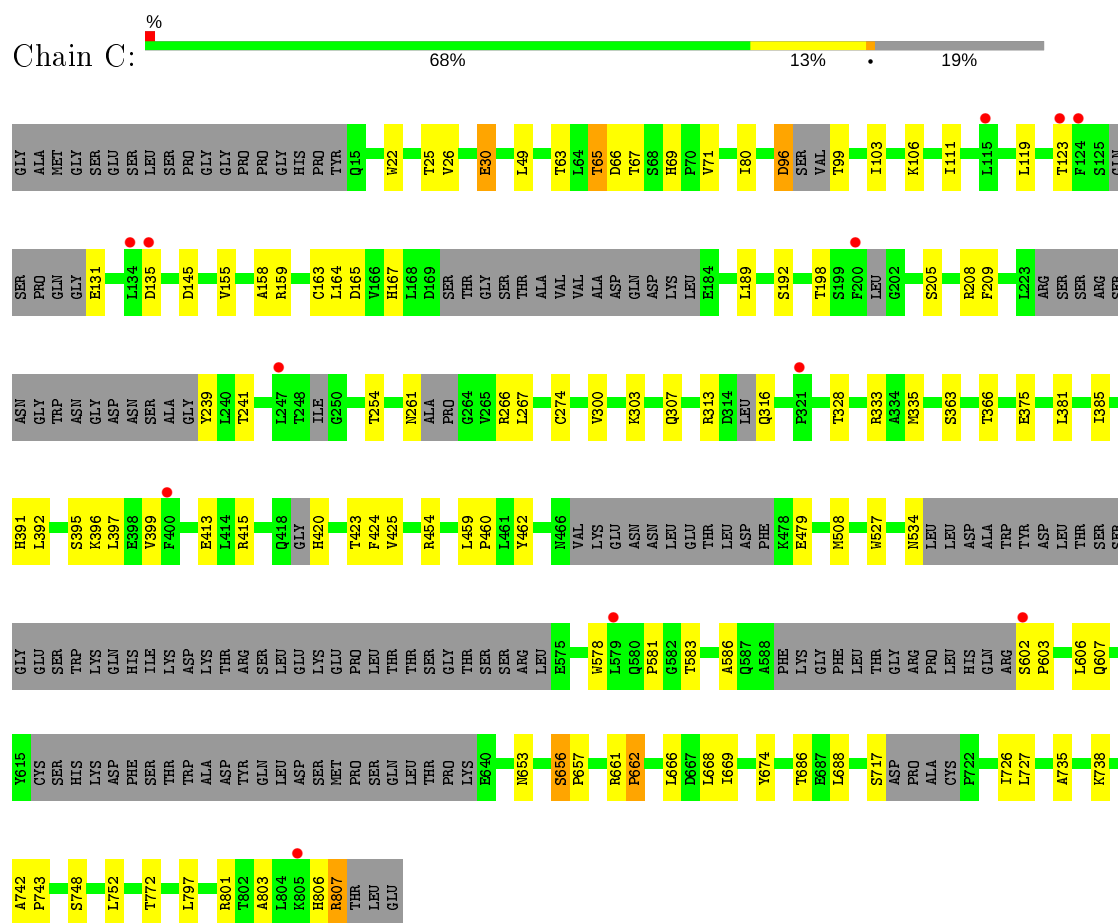


- Molecule 1: Cytosolic phospholipase A2 delta

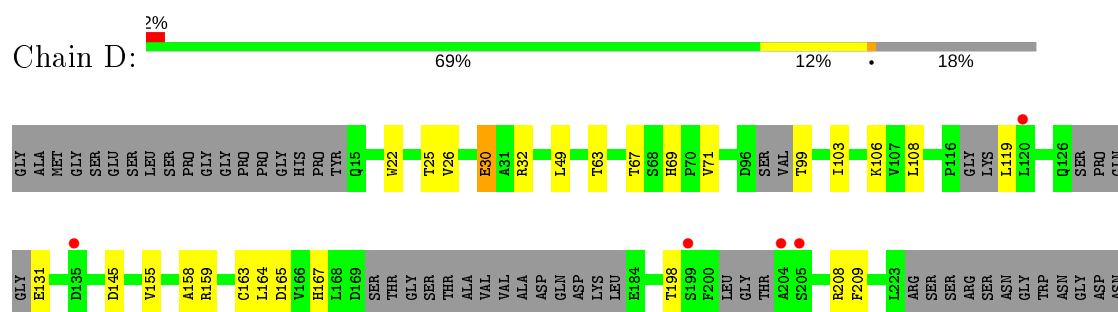


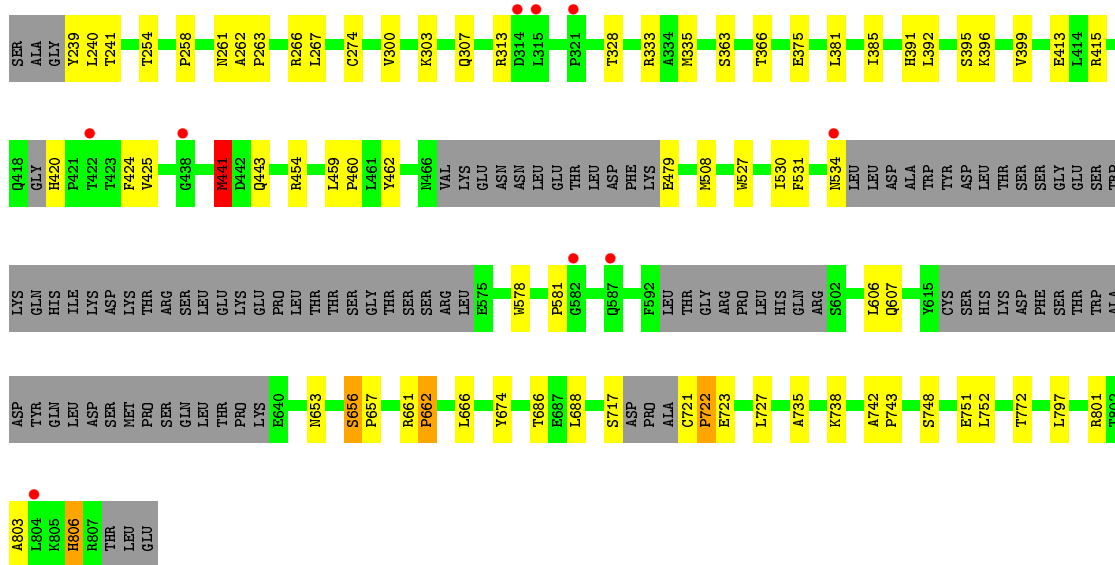


- Molecule 1: Cytosolic phospholipase A2 delta



- Molecule 1: Cytosolic phospholipase A2 delta





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.82Å 112.67Å 159.20Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	159.20 – 3.25 49.18 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (159.20-3.25) 99.5 (49.18-3.25)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.25Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.230 , 0.267 0.234 , 0.264	Depositor DCC
R_{free} test set	2849 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtrriage
Anisotropy	0.835	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.107 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21369	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3361e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7FA, TB

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	0.41	0/5487	0.64	1/7433 (0.0%)
1	B	0.43	0/5467	0.65	1/7411 (0.0%)
1	C	0.41	0/5354	0.64	0/7247
1	D	0.40	0/5406	0.64	1/7323 (0.0%)
All	All	0.42	0/21714	0.64	3/29414 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	ARG	N-CA-C	7.33	130.79	111.00
1	A	66	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	441	MET	CG-SD-CE	5.04	108.25	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5369	0	5301	46	3
1	B	5350	0	5245	47	3
1	C	5244	0	5156	50	1
1	D	5291	0	5204	48	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	22	0	34	1	0
2	B	22	0	34	0	0
2	C	22	0	34	0	0
2	D	22	0	34	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	3	0	0	0	0
3	D	4	0	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	5	0	0	0	0
All	All	21369	0	21042	191	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (191) 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:C:123:THR:HG22	1:C:135:ASP:OD1	1.69	0.93
1:B:536:LEU:HD21	1:B:641:PRO:HB2	1.57	0.84
1:A:391:HIS:O	1:A:396:LYS:NZ	2.24	0.71
1:D:391:HIS:O	1:D:396:LYS:NZ	2.24	0.71
1:B:391:HIS:O	1:B:396:LYS:NZ	2.25	0.70
1:C:391:HIS:O	1:C:396:LYS:NZ	2.24	0.70
1:D:240:LEU:HD11	1:D:258:PRO:CD	2.22	0.69
1:C:602:SER:N	1:C:603:PRO:HD3	2.07	0.69
1:D:159:ARG:N	1:D:508:MET:HE1	2.07	0.69
1:B:602:SER:N	1:B:603:PRO:HD3	2.08	0.68
1:C:159:ARG:N	1:C:508:MET:HE1	2.08	0.68
1:A:159:ARG:N	1:A:508:MET:HE1	2.08	0.68
1:A:262:ALA:HB1	1:A:263:PRO:CD	2.24	0.67
1:B:159:ARG:N	1:B:508:MET:HE1	2.10	0.67
1:D:530:ILE:HD11	1:D:531:PHE:CZ	2.29	0.67
1:D:262:ALA:HB1	1:D:263:PRO:CD	2.25	0.66
1:A:333:ARG:NH1	1:A:674:TYR:O	2.29	0.65
1:C:333:ARG:NH1	1:C:674:TYR:O	2.29	0.65
1:B:333:ARG:NH1	1:B:674:TYR:O	2.30	0.65
1:D:333:ARG:NH1	1:D:674:TYR:O	2.30	0.65
1:C:123:THR:CG2	1:C:135:ASP:OD1	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:SER:N	1:C:603:PRO:CD	2.60	0.63
1:D:240:LEU:CD1	1:D:258:PRO:HD2	2.30	0.62
1:B:602:SER:N	1:B:603:PRO:CD	2.63	0.61
1:A:262:ALA:HB1	1:A:263:PRO:HD2	1.83	0.61
1:D:262:ALA:HB1	1:D:263:PRO:HD2	1.85	0.59
1:C:96:ASP:OD1	1:C:96:ASP:C	2.42	0.58
1:A:415:ARG:O	1:A:420:HIS:HB2	2.05	0.57
1:A:189:LEU:O	1:A:192:SER:OG	2.23	0.56
1:D:240:LEU:CD1	1:D:258:PRO:CD	2.83	0.56
1:D:415:ARG:O	1:D:420:HIS:HB2	2.06	0.56
1:B:718:ASP:O	1:B:722:PRO:N	2.40	0.55
1:C:735:ALA:O	1:C:738:LYS:HG3	2.07	0.55
1:C:415:ARG:O	1:C:420:HIS:HB2	2.06	0.55
1:B:415:ARG:O	1:B:420:HIS:HB2	2.07	0.54
1:D:735:ALA:O	1:D:738:LYS:HG3	2.08	0.54
1:D:381:LEU:O	1:D:385:ILE:HG12	2.08	0.54
1:B:163:CYS:HB3	1:B:208:ARG:HD2	1.90	0.53
1:B:328:THR:O	1:B:363:SER:OG	2.26	0.53
1:C:307:GLN:OE1	1:C:307:GLN:N	2.40	0.53
1:A:328:THR:O	1:A:363:SER:OG	2.27	0.53
1:B:381:LEU:O	1:B:385:ILE:HG12	2.09	0.53
1:A:381:LEU:O	1:A:385:ILE:HG12	2.09	0.53
1:D:328:THR:O	1:D:363:SER:OG	2.27	0.53
1:A:307:GLN:OE1	1:A:307:GLN:N	2.41	0.53
1:C:328:THR:O	1:C:363:SER:OG	2.27	0.53
1:C:381:LEU:O	1:C:385:ILE:HG12	2.09	0.53
1:D:307:GLN:N	1:D:307:GLN:OE1	2.41	0.53
1:C:163:CYS:HB3	1:C:208:ARG:HD2	1.91	0.53
1:B:712:GLU:OE2	1:B:735:ALA:HB3	2.10	0.52
1:B:533:LEU:HD13	1:B:533:LEU:N	2.25	0.52
1:A:163:CYS:HB3	1:A:208:ARG:HD2	1.90	0.52
1:C:668:LEU:HD13	1:C:726:ILE:HB	1.90	0.52
1:A:303:LYS:O	1:A:307:GLN:OE1	2.27	0.52
1:D:303:LYS:O	1:D:307:GLN:OE1	2.27	0.52
1:D:163:CYS:HB3	1:D:208:ARG:HD2	1.91	0.52
1:A:712:GLU:OE2	1:A:735:ALA:HB3	2.10	0.52
1:A:158:ALA:C	1:A:508:MET:HE1	2.30	0.51
1:C:303:LYS:O	1:C:307:GLN:OE1	2.27	0.51
1:B:303:LYS:O	1:B:307:GLN:OE1	2.27	0.51
1:B:307:GLN:OE1	1:B:307:GLN:N	2.42	0.51
1:B:26:VAL:HG21	1:B:49:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:VAL:HG21	1:C:49:LEU:HD13	1.92	0.51
1:B:459:LEU:HD12	1:B:460:PRO:HD2	1.92	0.51
1:C:396:LYS:HE2	1:C:772:THR:HG22	1.92	0.51
1:D:240:LEU:HD11	1:D:258:PRO:HD3	1.93	0.51
1:D:30:GLU:HB3	1:D:71:VAL:HG22	1.92	0.51
1:C:459:LEU:HD12	1:C:460:PRO:HD2	1.92	0.51
1:A:184:GLU:N	1:A:200:PHE:HA	2.26	0.51
1:C:158:ALA:C	1:C:508:MET:HE1	2.30	0.51
1:D:158:ALA:C	1:D:508:MET:HE1	2.31	0.51
1:B:30:GLU:HB3	1:B:71:VAL:HG22	1.91	0.51
1:A:30:GLU:HB3	1:A:71:VAL:HG22	1.92	0.50
1:B:396:LYS:HE2	1:B:772:THR:HG22	1.93	0.50
1:D:26:VAL:HG21	1:D:49:LEU:HD13	1.92	0.50
1:D:459:LEU:HD12	1:D:460:PRO:HD2	1.92	0.50
1:A:26:VAL:HG21	1:A:49:LEU:HD13	1.93	0.50
1:A:396:LYS:HE2	1:A:772:THR:HG22	1.94	0.50
1:A:459:LEU:HD12	1:A:460:PRO:HD2	1.93	0.50
1:A:656:SER:N	1:A:657:PRO:CD	2.75	0.49
1:B:158:ALA:C	1:B:508:MET:HE1	2.32	0.49
1:D:396:LYS:HG2	1:D:772:THR:HG22	1.94	0.49
1:D:396:LYS:HE2	1:D:772:THR:HG22	1.94	0.49
1:A:32:ARG:HG2	1:A:69:HIS:CD2	2.47	0.49
1:A:396:LYS:HG2	1:A:772:THR:HG22	1.94	0.49
1:C:30:GLU:HB3	1:C:71:VAL:HG22	1.93	0.49
1:D:441:MET:HE2	1:D:443:GLN:HG3	1.94	0.49
1:B:536:LEU:HB3	1:B:537:ASP:HA	1.95	0.49
1:B:656:SER:N	1:B:657:PRO:CD	2.75	0.49
1:C:656:SER:N	1:C:657:PRO:CD	2.75	0.49
1:A:530:ILE:HD13	2:A:901:7FA:H4A	1.94	0.49
1:A:721:CYS:O	1:A:723:GLU:N	2.45	0.48
1:D:32:ARG:HG2	1:D:69:HIS:CD2	2.48	0.48
1:B:335:MET:HG3	1:B:366:THR:OG1	2.13	0.48
1:B:32:ARG:HG2	1:B:69:HIS:CD2	2.48	0.48
1:C:65:THR:HG22	1:C:66:ASP:OD1	2.14	0.48
1:C:803:ALA:O	1:C:806:HIS:HB3	2.13	0.48
1:A:165:ASP:OD2	1:A:167:HIS:NE2	2.42	0.48
1:B:375:GLU:OE2	1:B:454:ARG:NH2	2.46	0.48
1:D:721:CYS:O	1:D:723:GLU:N	2.45	0.48
1:C:396:LYS:HG2	1:C:772:THR:HG22	1.96	0.48
1:D:578:TRP:HA	1:D:581:PRO:HD2	1.95	0.48
1:D:656:SER:N	1:D:657:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:TRP:HA	1:A:581:PRO:HD2	1.95	0.48
1:A:335:MET:HG3	1:A:366:THR:OG1	2.14	0.48
1:C:335:MET:HG3	1:C:366:THR:OG1	2.14	0.48
1:B:396:LYS:HG2	1:B:772:THR:HG22	1.96	0.47
1:C:375:GLU:OE2	1:C:454:ARG:NH2	2.47	0.47
1:C:69:HIS:CD2	1:C:69:HIS:O	2.67	0.47
1:D:165:ASP:OD2	1:D:167:HIS:NE2	2.43	0.47
1:B:165:ASP:OD2	1:B:167:HIS:NE2	2.43	0.47
1:C:661:ARG:HG3	1:C:662:PRO:HD2	1.96	0.47
1:D:335:MET:HG3	1:D:366:THR:OG1	2.14	0.47
1:A:375:GLU:OE2	1:A:454:ARG:NH2	2.47	0.47
1:B:661:ARG:HG3	1:B:662:PRO:HD2	1.96	0.47
1:D:661:ARG:HG3	1:D:662:PRO:HD2	1.96	0.47
1:A:661:ARG:HG3	1:A:662:PRO:HD2	1.96	0.47
1:C:668:LEU:HD12	1:C:669:ILE:H	1.80	0.47
1:D:375:GLU:OE2	1:D:454:ARG:NH2	2.47	0.47
1:C:807:ARG:HD3	1:C:807:ARG:N	2.29	0.47
1:B:578:TRP:HA	1:B:581:PRO:HD2	1.96	0.46
1:C:165:ASP:OD2	1:C:167:HIS:NE2	2.44	0.46
1:D:530:ILE:CD1	1:D:531:PHE:CZ	2.97	0.46
1:C:578:TRP:HA	1:C:581:PRO:HD2	1.97	0.45
1:B:441:MET:HE2	1:B:443:GLN:HG3	1.98	0.45
1:C:668:LEU:HD12	1:C:669:ILE:N	2.31	0.45
1:C:392:LEU:O	1:C:772:THR:HA	2.16	0.45
1:D:392:LEU:O	1:D:772:THR:HA	2.17	0.45
1:A:103:ILE:HD11	1:A:106:LYS:HB2	1.99	0.45
1:B:392:LEU:O	1:B:772:THR:HA	2.16	0.45
1:C:266:ARG:O	1:C:267:LEU:HD23	2.17	0.45
1:B:266:ARG:O	1:B:267:LEU:HD23	2.17	0.44
1:D:103:ILE:HD11	1:D:106:LYS:HB2	1.99	0.44
1:A:163:CYS:HA	1:A:209:PHE:O	2.17	0.44
1:A:803:ALA:O	1:A:806:HIS:HB2	2.16	0.44
1:D:266:ARG:O	1:D:267:LEU:HD23	2.17	0.44
1:B:163:CYS:HA	1:B:209:PHE:O	2.18	0.44
1:A:266:ARG:O	1:A:267:LEU:HD23	2.17	0.44
1:A:392:LEU:O	1:A:772:THR:HA	2.18	0.44
1:D:131:GLU:HA	1:D:131:GLU:OE1	2.18	0.44
1:D:163:CYS:HA	1:D:209:PHE:O	2.18	0.43
1:B:103:ILE:HD11	1:B:106:LYS:HB2	1.99	0.43
1:A:661:ARG:CG	1:A:662:PRO:HD2	2.49	0.43
1:D:661:ARG:CG	1:D:662:PRO:HD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:803:ALA:O	1:D:806:HIS:HB2	2.18	0.43
1:C:103:ILE:HD11	1:C:106:LYS:HB2	1.99	0.43
1:C:661:ARG:CG	1:C:662:PRO:HD2	2.49	0.43
1:D:797:LEU:O	1:D:801:ARG:HG3	2.19	0.43
1:C:163:CYS:HA	1:C:209:PHE:O	2.19	0.43
1:A:797:LEU:O	1:A:801:ARG:HG3	2.19	0.43
1:B:797:LEU:O	1:B:801:ARG:HG3	2.19	0.43
1:B:661:ARG:CG	1:B:662:PRO:HD2	2.49	0.42
1:C:606:LEU:O	1:C:607:GLN:C	2.57	0.42
1:D:721:CYS:N	1:D:722:PRO:HD3	2.34	0.42
1:C:797:LEU:O	1:C:801:ARG:HG3	2.20	0.42
1:D:396:LYS:HG2	1:D:772:THR:CG2	2.50	0.42
1:A:396:LYS:HG2	1:A:772:THR:CG2	2.50	0.42
1:C:158:ALA:CA	1:C:508:MET:HE1	2.50	0.42
1:B:536:LEU:HD21	1:B:641:PRO:CB	2.40	0.42
1:B:158:ALA:CA	1:B:508:MET:HE1	2.50	0.42
1:A:153:ASN:ND2	1:A:493:TYR:O	2.53	0.41
1:A:742:ALA:HB1	1:A:743:PRO:HD2	2.02	0.41
1:C:80:ILE:HD12	1:C:111:ILE:HD11	2.02	0.41
1:C:583:THR:O	1:C:586:ALA:HB3	2.20	0.41
1:A:721:CYS:N	1:A:722:PRO:HD3	2.35	0.41
1:C:462:TYR:CD1	1:C:527:TRP:CZ3	3.08	0.41
1:C:396:LYS:HG2	1:C:772:THR:CG2	2.51	0.41
1:D:606:LEU:O	1:D:607:GLN:C	2.59	0.41
1:D:656:SER:HB3	1:D:686:THR:HG23	2.03	0.41
1:A:119:LEU:HD12	1:A:120:LEU:N	2.35	0.41
1:A:656:SER:HB3	1:A:686:THR:HG23	2.02	0.41
1:C:189:LEU:O	1:C:192:SER:OG	2.22	0.41
1:C:742:ALA:HB1	1:C:743:PRO:HD2	2.02	0.41
1:B:396:LYS:O	1:B:399:VAL:HG12	2.20	0.41
1:B:38:ASP:HB3	1:B:39:LEU:HD12	2.03	0.41
1:B:742:ALA:HB1	1:B:743:PRO:HD2	2.02	0.41
1:A:158:ALA:CA	1:A:508:MET:HE1	2.50	0.41
1:C:656:SER:HB3	1:C:686:THR:HG23	2.03	0.41
1:A:456:GLN:HG2	1:A:457:ASN:ND2	2.36	0.41
1:A:44:ASP:OD2	1:A:66:ASP:OD1	2.39	0.41
1:B:396:LYS:HG2	1:B:772:THR:CG2	2.51	0.41
1:D:742:ALA:HB1	1:D:743:PRO:HD2	2.03	0.41
1:A:34:LEU:HB2	1:A:68:SER:HA	2.03	0.40
1:B:656:SER:HB3	1:B:686:THR:HG23	2.03	0.40
1:C:396:LYS:O	1:C:399:VAL:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:O	1:B:192:SER:OG	2.23	0.40
1:B:536:LEU:CB	1:B:537:ASP:HA	2.51	0.40
1:D:462:TYR:CD1	1:D:527:TRP:CZ3	3.10	0.40
1:B:414:LEU:O	1:B:418:GLN:OE1	2.40	0.40
1:B:80:ILE:HD12	1:B:111:ILE:HD11	2.03	0.40
1:D:396:LYS:O	1:D:399:VAL:HG12	2.20	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLU:OE1	1:B:699:ARG:NH2[1_565]	1.92	0.28
1:C:165:ASP:OD2	1:D:165:ASP:OD2[2_355]	2.00	0.20
1:A:165:ASP:OD2	1:B:165:ASP:OD2[2_456]	2.02	0.18
1:A:38:ASP:OD1	1:B:642:ARG:O[2_556]	2.07	0.13

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	654/814 (80%)	616 (94%)	35 (5%)	3 (0%)	29	62
1	B	653/814 (80%)	615 (94%)	36 (6%)	2 (0%)	41	72
1	C	629/814 (77%)	594 (94%)	34 (5%)	1 (0%)	47	77
1	D	638/814 (78%)	603 (94%)	33 (5%)	2 (0%)	41	72
All	All	2574/3256 (79%)	2428 (94%)	138 (5%)	8 (0%)	41	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	662	PRO

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Mol	Chain	Res	Type
1	B	662	PRO
1	C	662	PRO
1	D	662	PRO
1	A	722	PRO
1	A	419	GLY
1	D	722	PRO
1	B	419	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	584/705 (83%)	545 (93%)	39 (7%)	16	45
1	B	581/705 (82%)	546 (94%)	35 (6%)	19	49
1	C	571/705 (81%)	531 (93%)	40 (7%)	15	43
1	D	576/705 (82%)	540 (94%)	36 (6%)	18	47
All	All	2312/2820 (82%)	2162 (94%)	150 (6%)	17	46

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	TRP
1	A	25	THR
1	A	30	GLU
1	A	63	THR
1	A	67	THR
1	A	99	THR
1	A	108	LEU
1	A	119	LEU
1	A	131	GLU
1	A	145	ASP
1	A	155	VAL
1	A	164	LEU
1	A	198	THR
1	A	200	PHE

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Mol	Chain	Res	Type
1	A	216	GLU
1	A	239	TYR
1	A	241	THR
1	A	254	THR
1	A	261	ASN
1	A	274	CYS
1	A	300	VAL
1	A	313	ARG
1	A	395	SER
1	A	413	GLU
1	A	424	PHE
1	A	425	VAL
1	A	479	GLU
1	A	530	ILE
1	A	534	ASN
1	A	653	ASN
1	A	656	SER
1	A	666	LEU
1	A	688	LEU
1	A	717	SER
1	A	727	LEU
1	A	748	SER
1	A	751	GLU
1	A	752	LEU
1	A	806	HIS
1	B	22	TRP
1	B	25	THR
1	B	30	GLU
1	B	63	THR
1	B	67	THR
1	B	99	THR
1	B	119	LEU
1	B	131	GLU
1	B	145	ASP
1	B	155	VAL
1	B	164	LEU
1	B	198	THR
1	B	239	TYR
1	B	241	THR
1	B	254	THR
1	B	261	ASN
1	B	274	CYS

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Mol	Chain	Res	Type
1	B	300	VAL
1	B	313	ARG
1	B	413	GLU
1	B	423	THR
1	B	424	PHE
1	B	425	VAL
1	B	441	MET
1	B	479	GLU
1	B	530	ILE
1	B	533	LEU
1	B	653	ASN
1	B	656	SER
1	B	666	LEU
1	B	688	LEU
1	B	723	GLU
1	B	727	LEU
1	B	748	SER
1	B	752	LEU
1	C	22	TRP
1	C	25	THR
1	C	30	GLU
1	C	63	THR
1	C	65	THR
1	C	67	THR
1	C	96	ASP
1	C	99	THR
1	C	119	LEU
1	C	131	GLU
1	C	145	ASP
1	C	155	VAL
1	C	164	LEU
1	C	198	THR
1	C	205	SER
1	C	239	TYR
1	C	241	THR
1	C	254	THR
1	C	261	ASN
1	C	274	CYS
1	C	300	VAL
1	C	313	ARG
1	C	316	GLN
1	C	395	SER

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Mol	Chain	Res	Type
1	C	397	LEU
1	C	413	GLU
1	C	423	THR
1	C	424	PHE
1	C	425	VAL
1	C	479	GLU
1	C	534	ASN
1	C	653	ASN
1	C	656	SER
1	C	666	LEU
1	C	688	LEU
1	C	717	SER
1	C	727	LEU
1	C	748	SER
1	C	752	LEU
1	C	807	ARG
1	D	22	TRP
1	D	25	THR
1	D	30	GLU
1	D	63	THR
1	D	67	THR
1	D	99	THR
1	D	108	LEU
1	D	119	LEU
1	D	145	ASP
1	D	155	VAL
1	D	164	LEU
1	D	198	THR
1	D	239	TYR
1	D	241	THR
1	D	254	THR
1	D	261	ASN
1	D	274	CYS
1	D	300	VAL
1	D	313	ARG
1	D	395	SER
1	D	413	GLU
1	D	424	PHE
1	D	425	VAL
1	D	441	MET
1	D	479	GLU
1	D	534	ASN

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Mol	Chain	Res	Type
1	D	653	ASN
1	D	656	SER
1	D	666	LEU
1	D	688	LEU
1	D	717	SER
1	D	727	LEU
1	D	748	SER
1	D	751	GLU
1	D	752	LEU
1	D	806	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	443	GLN
1	C	69	HIS
1	D	443	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 15 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	7FA	B	901	1	18,21,22	0.26	0	16,21,24	0.65	0
2	7FA	C	901	1	18,21,22	0.25	0	16,21,24	0.66	0
2	7FA	A	901	1	18,21,22	0.36	0	16,21,24	0.58	0
2	7FA	D	901	1	18,21,22	0.25	0	16,21,24	0.56	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	7FA	B	901	1	-	5/16/20/22	-
2	7FA	C	901	1	-	7/16/20/22	-
2	7FA	A	901	1	-	7/16/20/22	-
2	7FA	D	901	1	-	3/16/20/22	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	7FA	C3-C4-C5-C6
2	C	901	7FA	C13-C14-C15-C16
2	D	901	7FA	C3-C4-C5-C6
2	A	901	7FA	C3-C4-C5-C6
2	B	901	7FA	C6-C7-C8-C9
2	D	901	7FA	C6-C7-C8-C9
2	C	901	7FA	C6-C7-C8-C9
2	C	901	7FA	C3-C4-C5-C6
2	A	901	7FA	C13-C14-C15-C16
2	A	901	7FA	C12-C13-C14-C15
2	D	901	7FA	C12-C13-C14-C15
2	C	901	7FA	C12-C13-C14-C15
2	C	901	7FA	C9-C10-C11-C12
2	A	901	7FA	C6-C7-C8-C9
2	A	901	7FA	C9-C10-C11-C12

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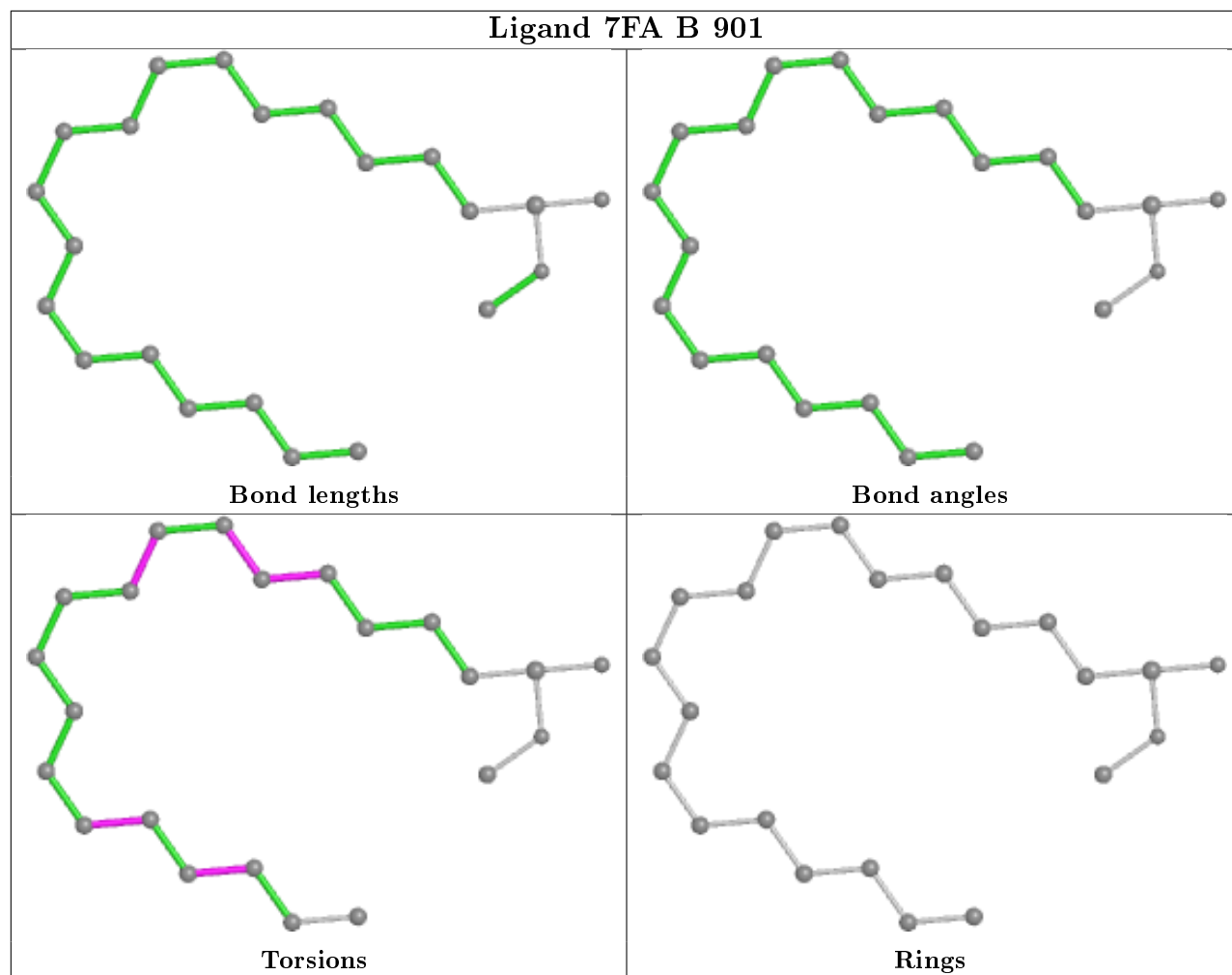
Mol	Chain	Res	Type	Atoms
2	B	901	7FA	C4-C5-C6-C7
2	A	901	7FA	C14-C15-C16-C17
2	B	901	7FA	C12-C13-C14-C15
2	A	901	7FA	C4-C5-C6-C7
2	C	901	7FA	C4-C5-C6-C7
2	B	901	7FA	C14-C15-C16-C17
2	C	901	7FA	C2-C3-C4-C5

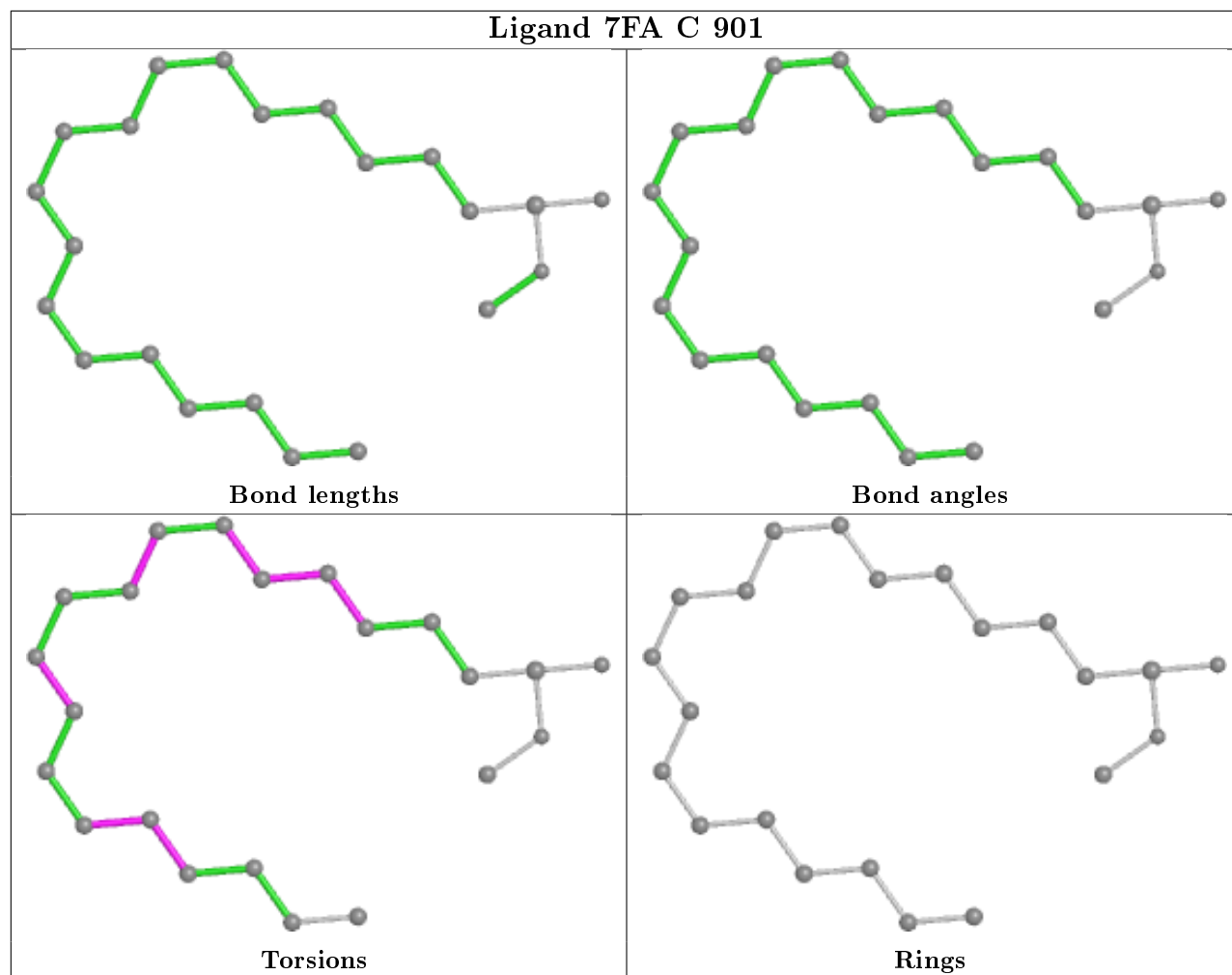
There are no ring outliers.

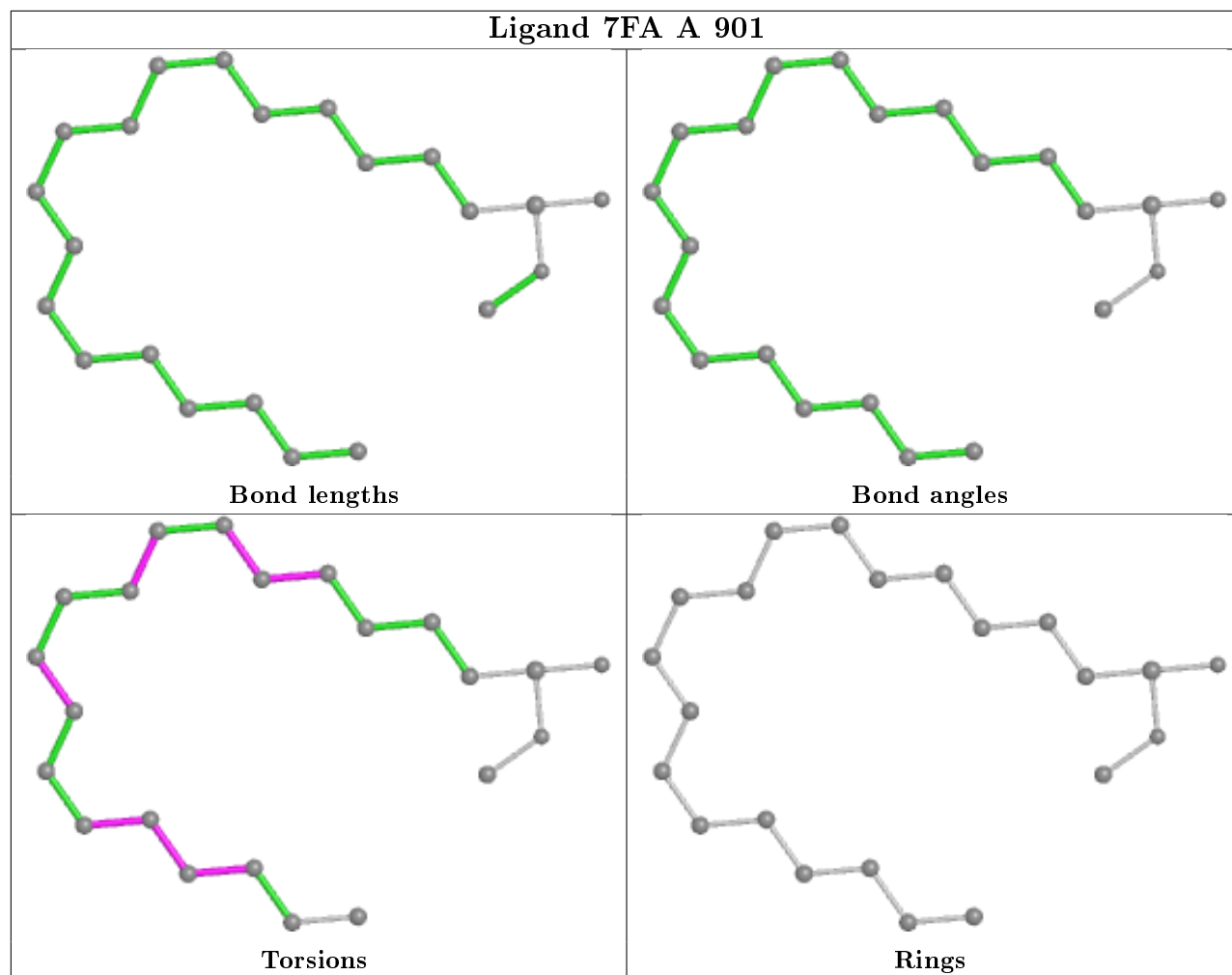
1 monomer is involved in 1 short contact:

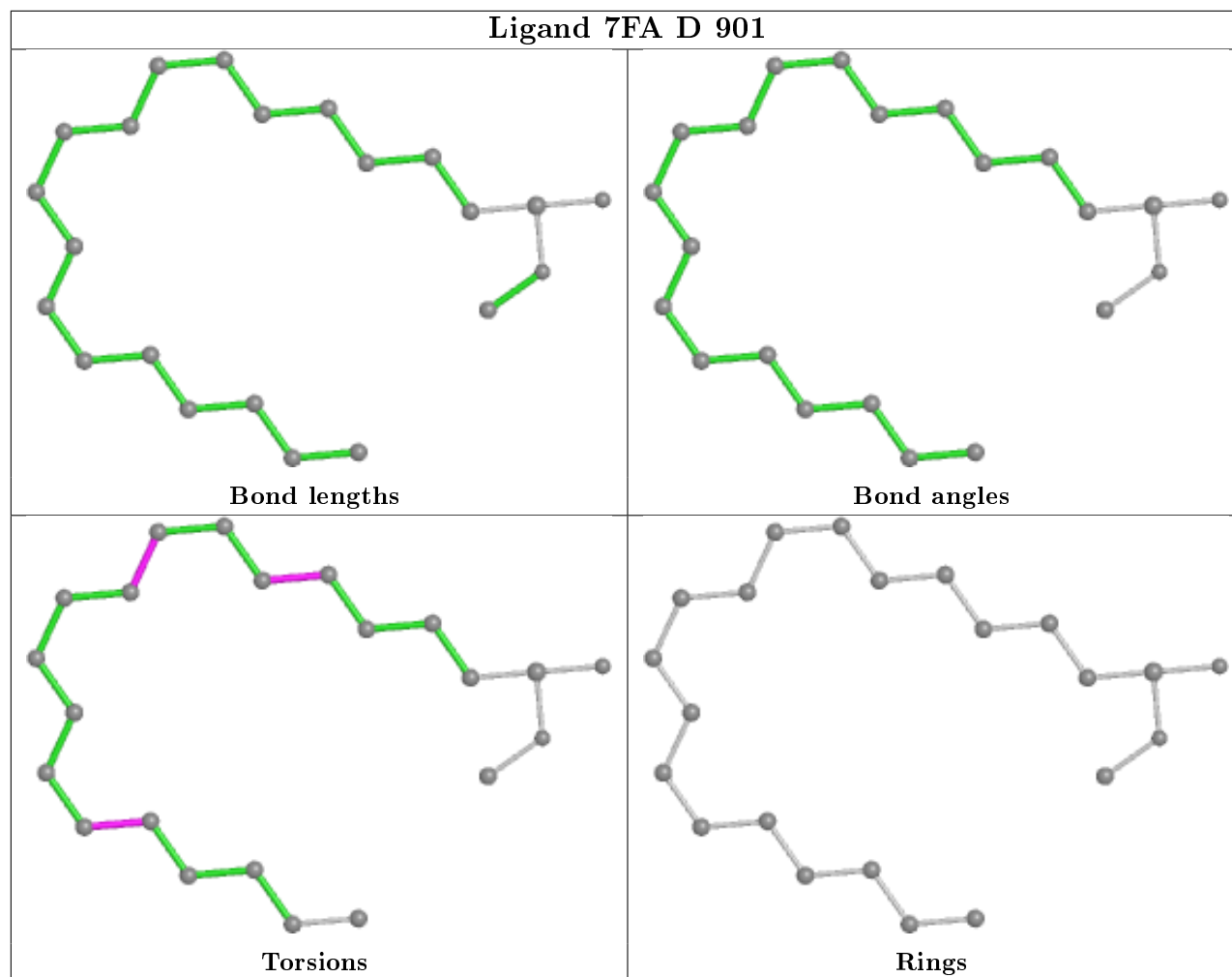
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	7FA	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	674/814 (82%)	-0.03	11 (1%) 72 69	42, 77, 124, 152	0
1	B	675/814 (82%)	-0.04	9 (1%) 77 75	44, 75, 123, 172	0
1	C	659/814 (80%)	0.02	12 (1%) 68 65	57, 89, 128, 149	0
1	D	664/814 (81%)	0.06	14 (2%) 63 61	53, 88, 134, 159	0
All	All	2672/3256 (82%)	0.00	46 (1%) 70 67	42, 83, 129, 172	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	VAL	6.2
1	A	203	THR	4.7
1	B	575	GLU	4.1
1	B	97	SER	3.7
1	D	315	LEU	3.5
1	B	442	ASP	3.4
1	D	321	PRO	3.4
1	D	204	ALA	3.2
1	A	312	ASP	3.1
1	D	314	ASP	3.0
1	A	118	LYS	3.0
1	A	169	ASP	2.9
1	B	120	LEU	2.9
1	C	400	PHE	2.8
1	D	438	GLY	2.8
1	D	205	SER	2.8
1	D	199	SER	2.8
1	C	579	LEU	2.7
1	C	321	PRO	2.7
1	A	315	LEU	2.7
1	A	200	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	113	GLU	2.6
1	C	135	ASP	2.6
1	D	804	LEU	2.6
1	A	97	SER	2.6
1	A	802	THR	2.6
1	C	123	THR	2.6
1	C	200	PHE	2.5
1	D	582	GLY	2.5
1	B	99	THR	2.5
1	C	115	LEU	2.4
1	C	124	PHE	2.4
1	C	134	LEU	2.4
1	D	120	LEU	2.3
1	C	805	LYS	2.3
1	B	131	GLU	2.3
1	D	422	THR	2.2
1	C	247	LEU	2.2
1	A	314	ASP	2.2
1	B	422	THR	2.1
1	D	135	ASP	2.1
1	C	602	SER	2.1
1	D	587	GLN	2.1
1	B	200	PHE	2.0
1	A	201	LEU	2.0
1	D	534	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

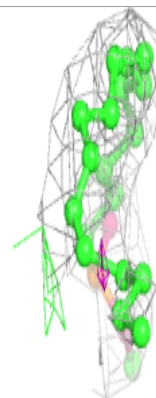
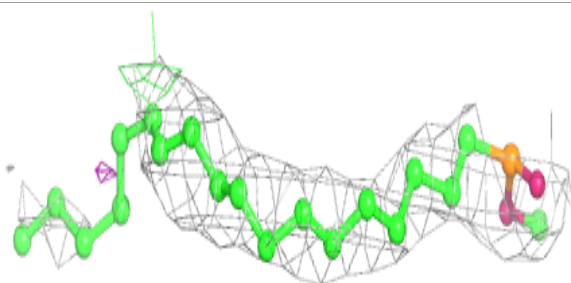
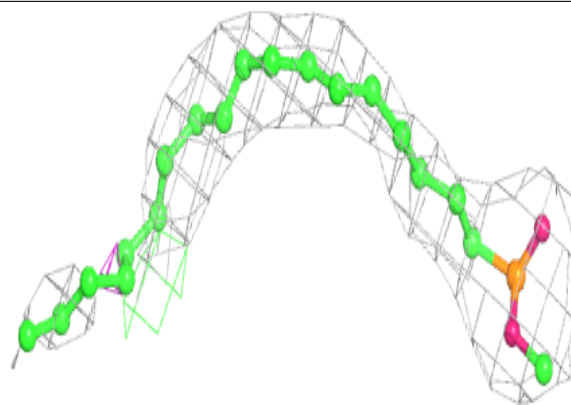
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TB	B	905	1/1	0.73	0.31	195,195,195,195	0
3	TB	C	904	1/1	0.82	0.22	146,146,146,146	0
3	TB	D	905	1/1	0.82	0.33	203,203,203,203	0
3	TB	A	905	1/1	0.85	0.36	175,175,175,175	0
3	TB	B	904	1/1	0.87	0.26	157,157,157,157	0
3	TB	D	903	1/1	0.88	0.15	130,130,130,130	0
2	7FA	A	901	22/23	0.89	0.39	55,66,93,104	0
3	TB	C	903	1/1	0.90	0.11	124,124,124,124	0
2	7FA	D	901	22/23	0.91	0.63	71,97,130,131	0
2	7FA	C	901	22/23	0.91	0.50	66,92,152,158	0
2	7FA	B	901	22/23	0.94	0.53	59,94,135,138	0
3	TB	A	903	1/1	0.95	0.11	125,125,125,125	0
3	TB	D	904	1/1	0.95	0.17	124,124,124,124	0
3	TB	A	904	1/1	0.96	0.21	122,122,122,122	0
3	TB	B	903	1/1	0.96	0.14	116,116,116,116	0
3	TB	C	902	1/1	0.97	0.07	95,95,95,95	0
3	TB	A	902	1/1	0.98	0.07	94,94,94,94	0
3	TB	D	902	1/1	0.98	0.07	96,96,96,96	0
3	TB	B	902	1/1	0.98	0.06	80,80,80,80	0

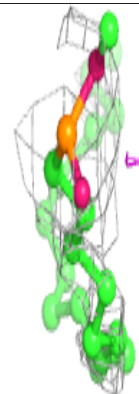
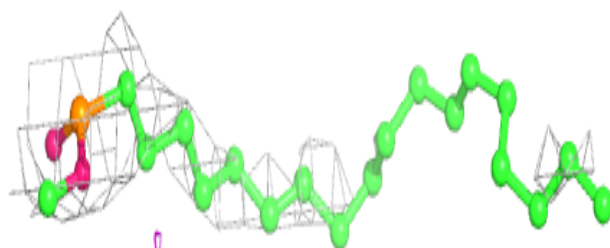
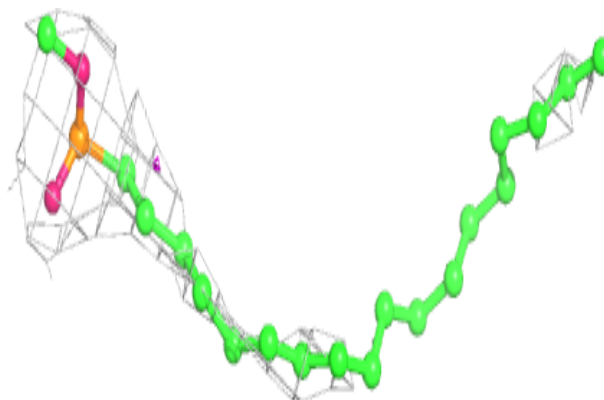
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7FA A 901:

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

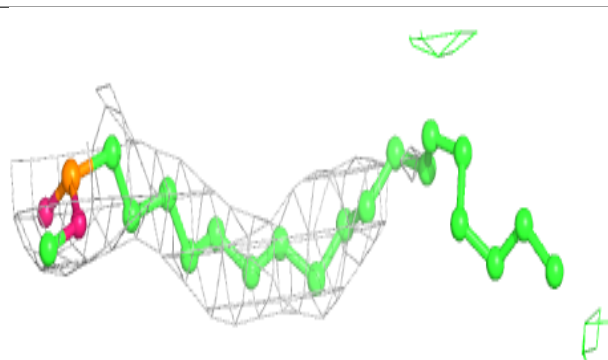
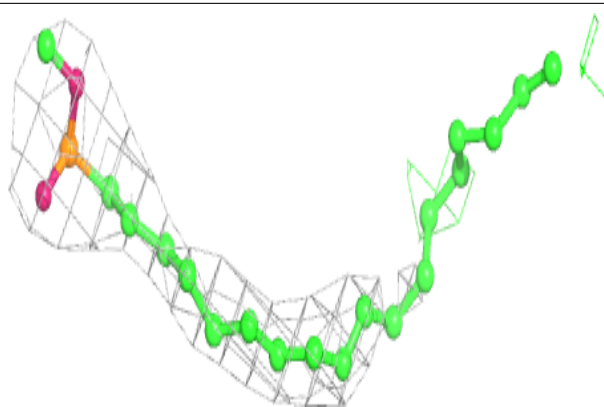
**Electron density around 7FA D 901:**

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

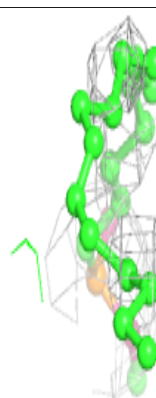
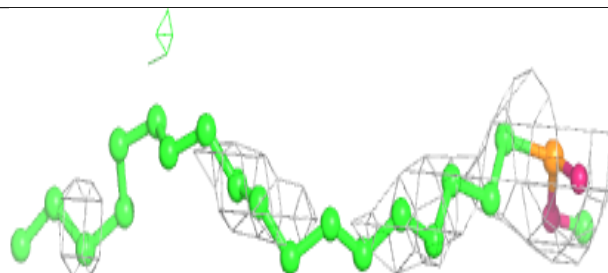
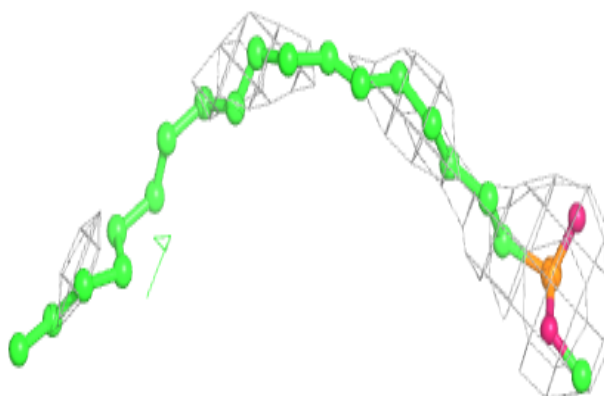


Electron density around 7FA C 901:

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

**Electron density around 7FA B 901:**

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



6.5 Other polymers

There are no such residues in this entry.