Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2024 – 07:39 AM EDT

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

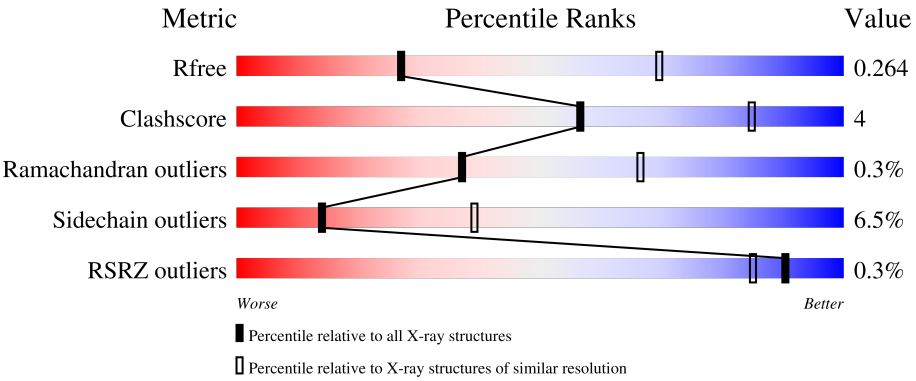
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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}	164625	1482 (3.30-3.22)
Clashscore	180529	1546 (3.30-3.22)
Ramachandran outliers	177936	1536 (3.30-3.22)
Sidechain outliers	177891	1535 (3.30-3.22)
RSRZ outliers	164620	1483 (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 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	814	69% 12% • 17%
1	B	814	70% 12% • 17%
1	C	814	68% 13% • 19%
1	D	814	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.

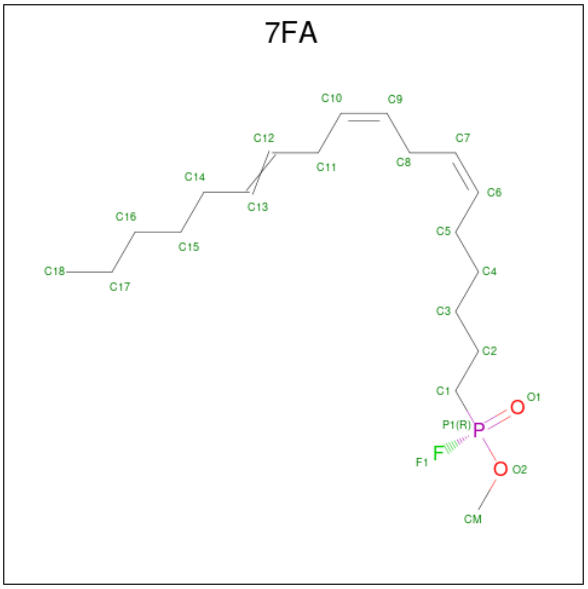
- Molecule 1 is a protein called Cytosolic phospholipase A2 delta.

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

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: $C_{19}H_{34}FO_2P$).



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

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

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

- Molecule 4 is water.

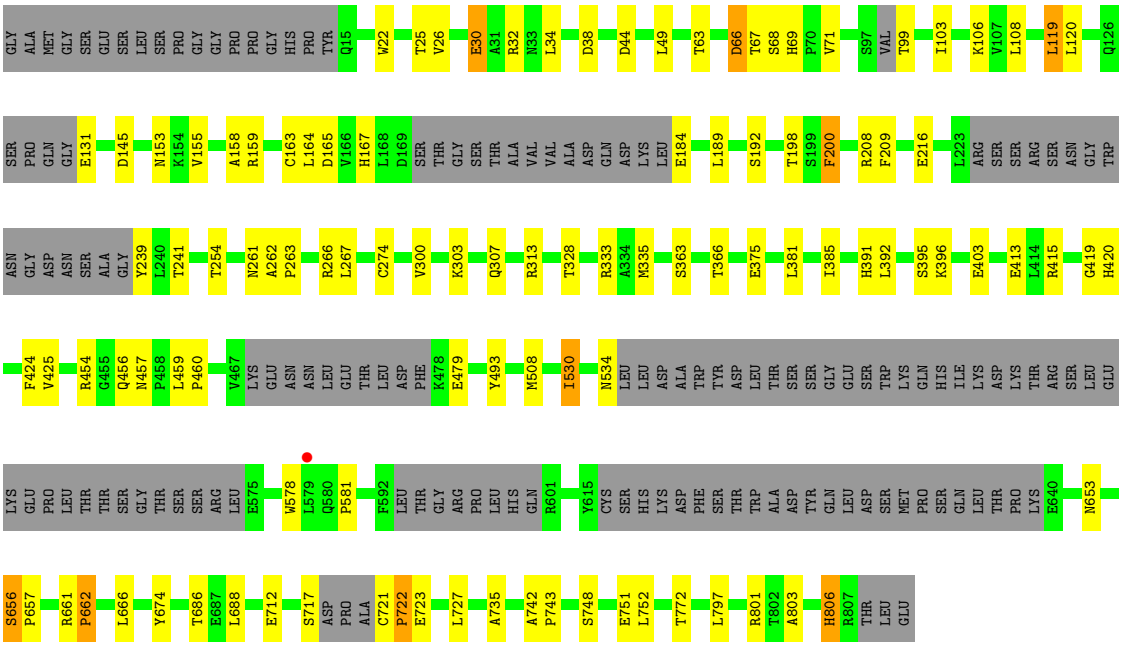
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	2	Total O 2 2	0	0
4	C	2	Total O 2 2	0	0
4	D	5	Total O 5 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

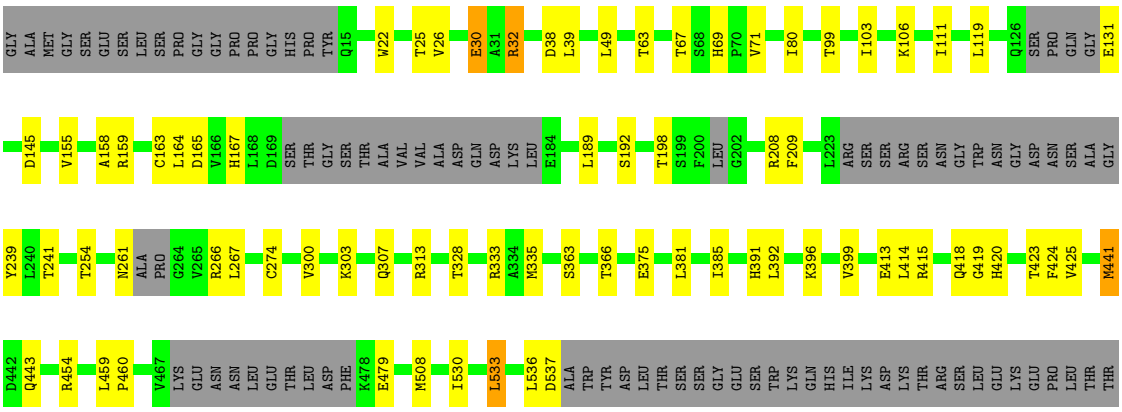
• Molecule 1: Cytosolic phospholipase A2 delta

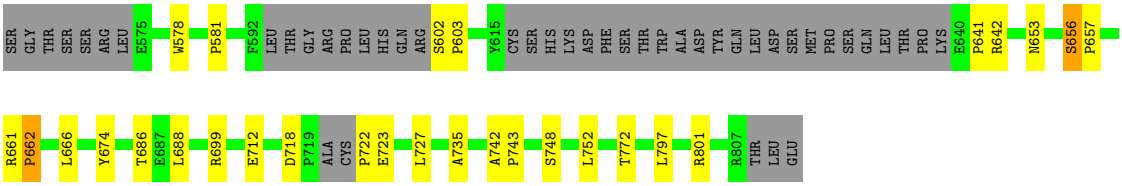
Chain A:



• Molecule 1: Cytosolic phospholipase A2 delta

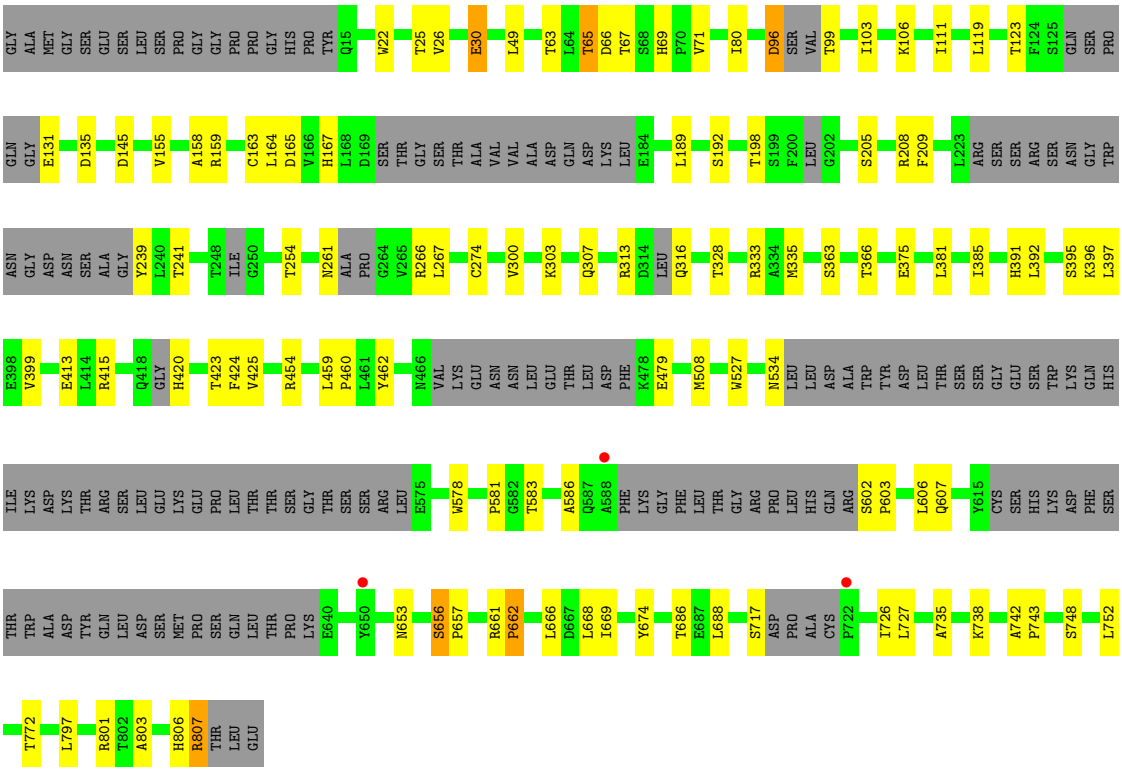
Chain B:





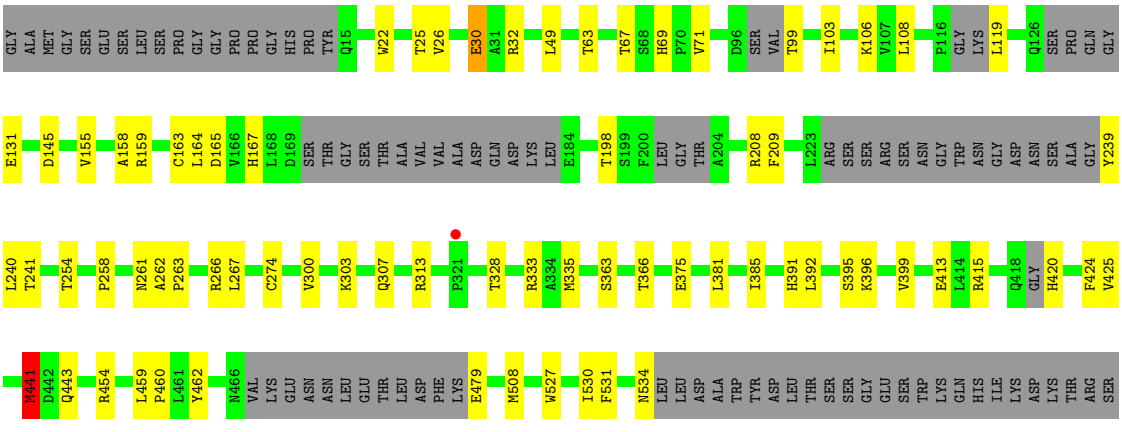
• Molecule 1: Cytosolic phospholipase A2 delta

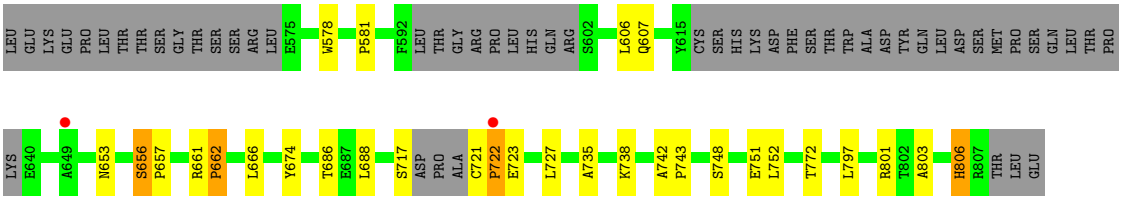
Chain C:



• Molecule 1: Cytosolic phospholipase A2 delta

Chain D:




LEU GLU LYS GLU PRO LEU THR THR SER GLY THR SER SER ARG LEU E575 W578 P581 F592 LEU THR GLY ARG PRO LEU HIS GLN ARG S602 L606 Q607 Y615 CYS SER HIS LYS ASP PHE SER THR TRP ALA ASP TYR GLN LEU ASP SER MET PRO SER GLN LEU THR PRO
LYS E640 A649 N653 S656 P657 R661 P662 L666 Y674 T686 E687 L688 S717 ASP PRO ALA C721 P722 E723 L727 A735 K738 A742 P743 S748 E751 L752 T772 L797 R801 T802 A803 H806 R807 THR LEU GLU

4 Data and refinement statistics (i)

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 – 3.25 159.20 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (159.20-3.25) 99.5 (159.20-3.25)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 3.25Å)	Xtriage
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	Xtriage
Anisotropy	0.835	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.107 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21369	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage'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.*

[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

5.1 Standard geometry

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

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(^{o})	Ideal(^{o})
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

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:N	1:A:307:GLN:OE1	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:N	1:B:533:LEU:HD13	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:30:GLU:HB3	1:D:71:VAL:HG22	1.92	0.51
1:D:240:LEU:HD11	1:D:258:PRO:HD3	1.93	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:69:HIS:CD2	1:C:69:HIS:O	2.67	0.47
1:C:375:GLU:OE2	1:C:454:ARG:NH2	2.47	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: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:D:661:ARG:HG3	1:D:662:PRO:HD2	1.96	0.47
1:C:807:ARG:N	1:C:807:ARG:HD3	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:396:LYS:HG2	1:C:772:THR:CG2	2.51	0.41
1:C:462:TYR:CD1	1:C:527:TRP:CZ3	3.08	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:38:ASP:HB3	1:B:39:LEU:HD12	2.03	0.41
1:B:396:LYS:O	1:B:399:VAL:HG12	2.20	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:44:ASP:OD2	1:A:66:ASP:OD1	2.39	0.41
1:A:456:GLN:HG2	1:A:457:ASN:ND2	2.36	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:80:ILE:HD12	1:B:111:ILE:HD11	2.03	0.40
1:B:414:LEU:O	1:B:418:GLN:OE1	2.40	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%)	25	56
1	B	653/814 (80%)	615 (94%)	36 (6%)	2 (0%)	37	66
1	C	629/814 (77%)	594 (94%)	34 (5%)	1 (0%)	44	71
1	D	638/814 (78%)	603 (94%)	33 (5%)	2 (0%)	37	66
All	All	2574/3256 (79%)	2428 (94%)	138 (5%)	8 (0%)	37	66

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%)	13	38
1	B	581/705 (82%)	546 (94%)	35 (6%)	16	41
1	C	571/705 (81%)	531 (93%)	40 (7%)	12	36
1	D	576/705 (82%)	540 (94%)	36 (6%)	15	40
All	All	2312/2820 (82%)	2162 (94%)	150 (6%)	14	39

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

Sometimes 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 oligosaccharides 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	C	901	1	18,21,22	0.25	0	16,21,24	0.58	0
2	7FA	D	901	1	18,21,22	0.25	0	16,21,24	0.53	0
2	7FA	B	901	1	18,21,22	0.26	0	16,21,24	0.58	0
2	7FA	A	901	1	18,21,22	0.37	0	16,21,24	0.55	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	C	901	1	-	7/16/20/22	-
2	7FA	D	901	1	-	3/16/20/22	-
2	7FA	B	901	1	-	5/16/20/22	-
2	7FA	A	901	1	-	7/16/20/22	-

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	A	901	7FA	C3-C4-C5-C6
2	D	901	7FA	C3-C4-C5-C6
2	C	901	7FA	C3-C4-C5-C6
2	B	901	7FA	C6-C7-C8-C9
2	C	901	7FA	C6-C7-C8-C9
2	D	901	7FA	C6-C7-C8-C9
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	A	901	7FA	C6-C7-C8-C9
2	A	901	7FA	C9-C10-C11-C12
2	C	901	7FA	C9-C10-C11-C12
2	C	901	7FA	C12-C13-C14-C15

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

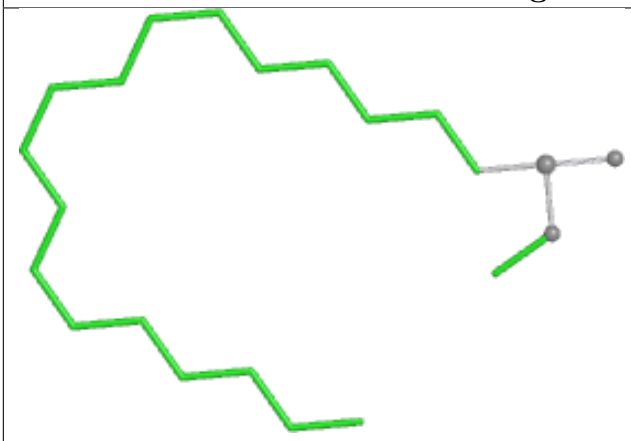
There are no ring outliers.

1 monomer is involved in 1 short contact:

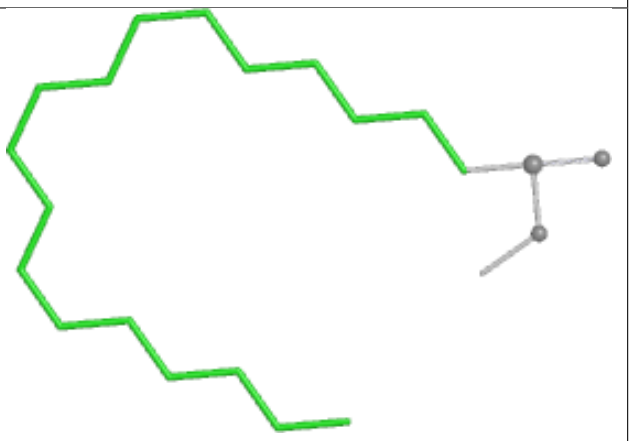
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	7FA	1	0

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 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.

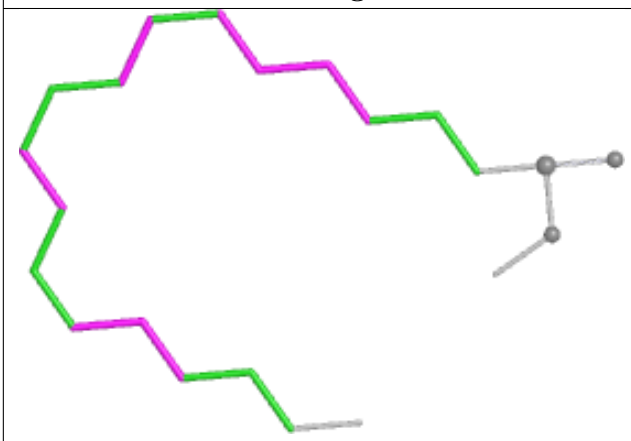
Ligand 7FA C 901



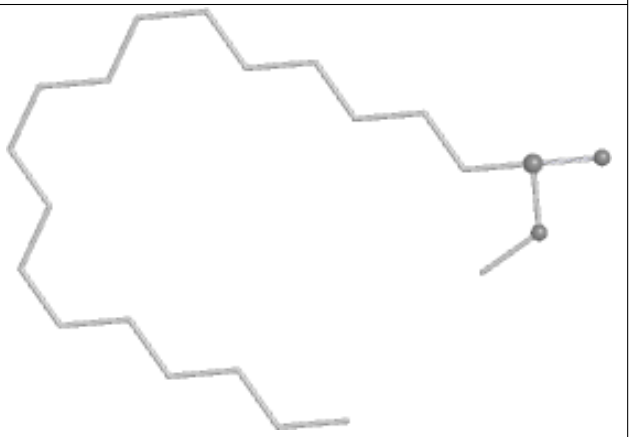
Bond lengths



Bond angles

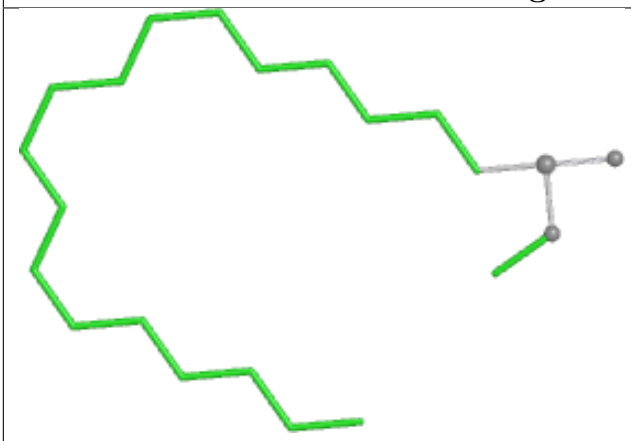


Torsions

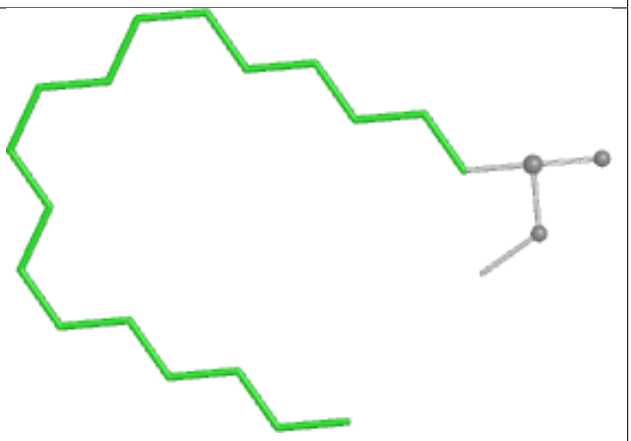


Rings

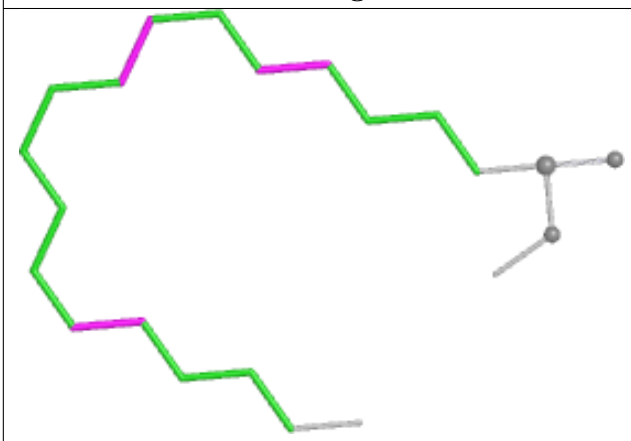
Ligand 7FA D 901



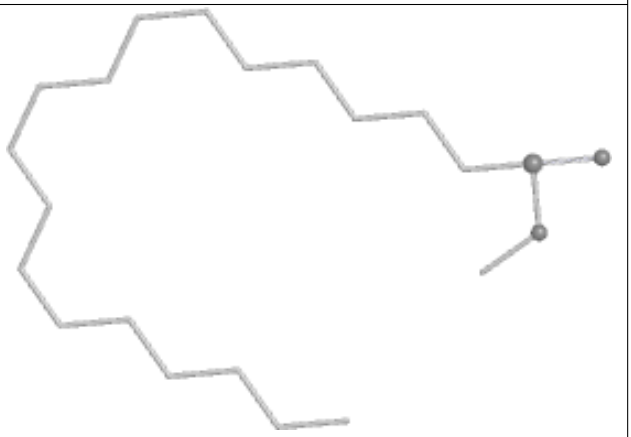
Bond lengths



Bond angles

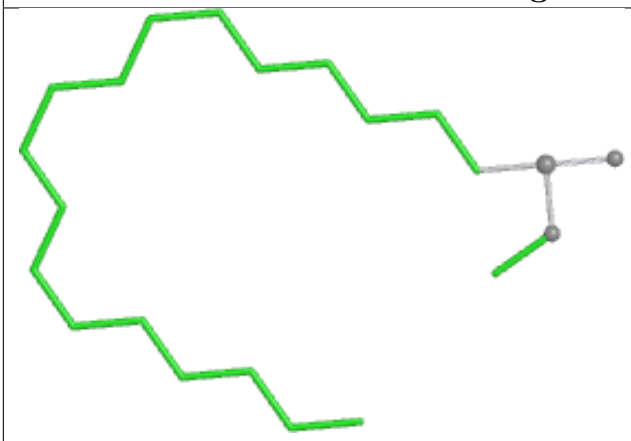


Torsions



Rings

Ligand 7FA B 901



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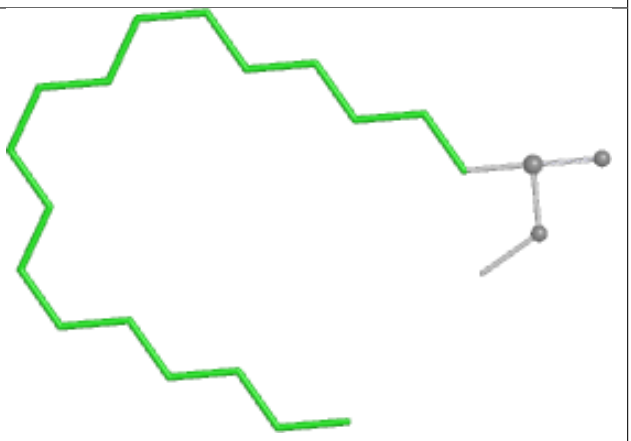

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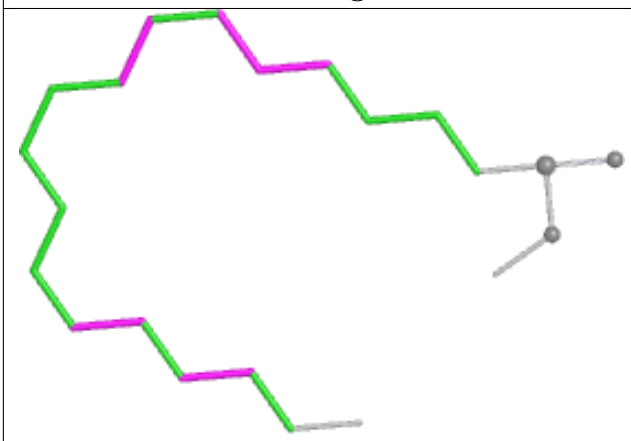

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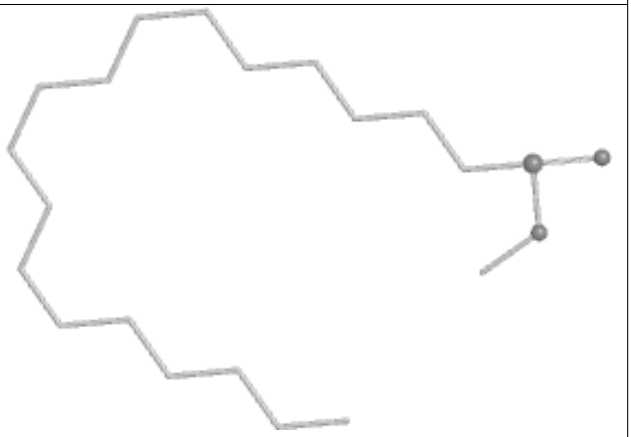
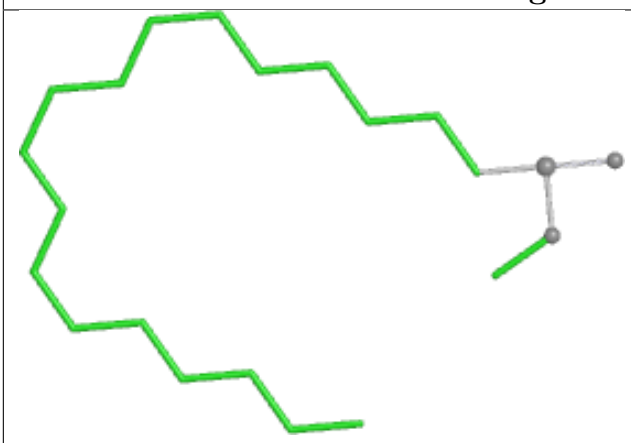


Rings

Ligand 7FA A 901



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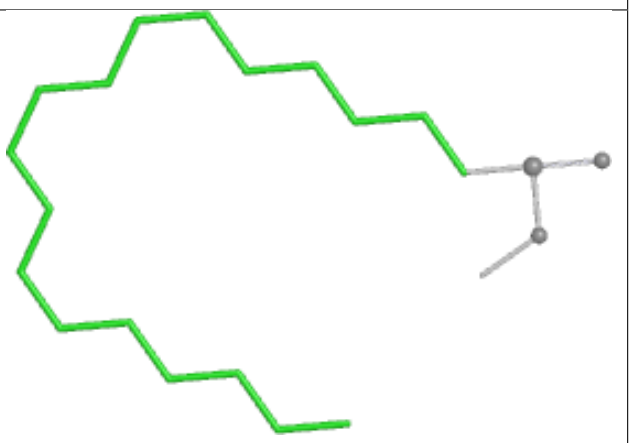

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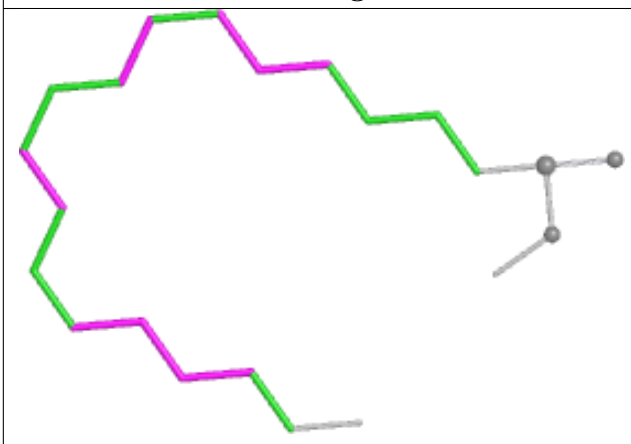

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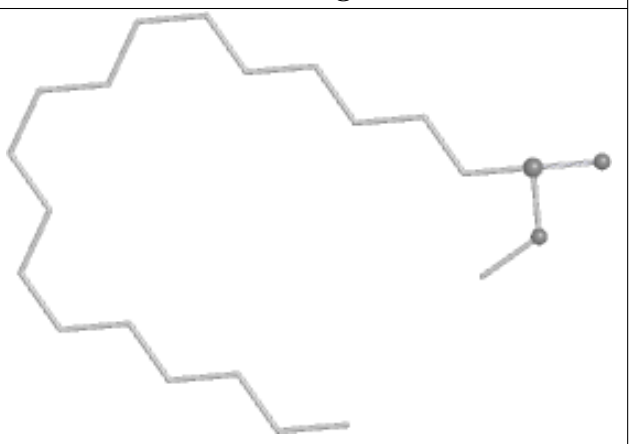


Rings

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, 95^{th} 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%)	-0.32	1 (0%) 92 91	42, 77, 124, 152	0
1	B	675/814 (82%)	-0.29	0 100 100	44, 75, 123, 172	0
1	C	659/814 (80%)	-0.24	3 (0%) 87 80	57, 89, 128, 149	0
1	D	664/814 (81%)	-0.25	3 (0%) 87 80	53, 88, 134, 159	0
All	All	2672/3256 (82%)	-0.28	7 (0%) 90 85	42, 83, 129, 172	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	722	PRO	3.0
1	C	588	ALA	2.6
1	C	650	TYR	2.3
1	D	321	PRO	2.3
1	A	579	LEU	2.2
1	C	722	PRO	2.1
1	D	649	ALA	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 (i)

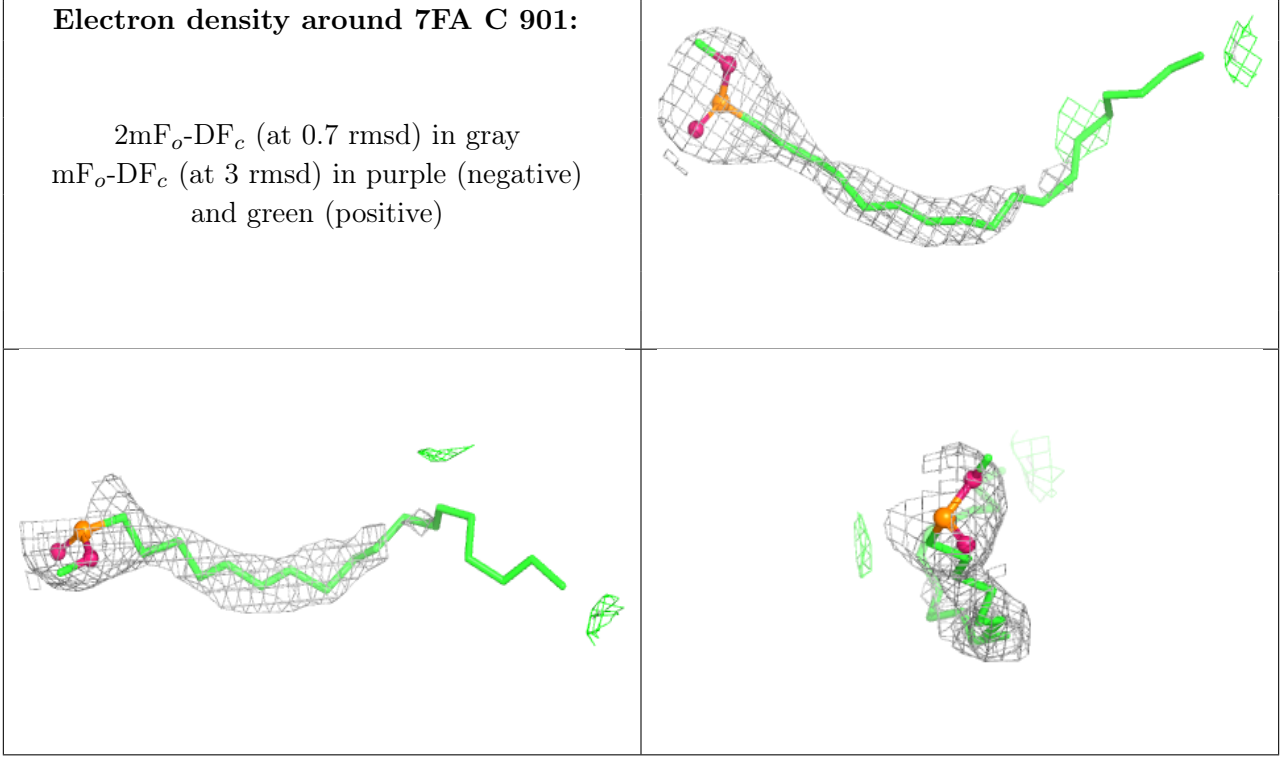
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TB	A	905	1/1	0.76	0.11	175,175,175,175	0
3	TB	B	905	1/1	0.76	0.08	195,195,195,195	0
3	TB	D	905	1/1	0.82	0.10	203,203,203,203	0
2	7FA	C	901	22/23	0.92	0.20	66,92,152,158	0
2	7FA	A	901	22/23	0.92	0.17	55,66,93,104	0
2	7FA	D	901	22/23	0.93	0.17	71,97,130,131	0
3	TB	C	904	1/1	0.94	0.05	146,146,146,146	0
2	7FA	B	901	22/23	0.94	0.18	59,94,135,138	0
3	TB	D	903	1/1	0.95	0.06	130,130,130,130	0
3	TB	D	904	1/1	0.95	0.05	124,124,124,124	0
3	TB	B	904	1/1	0.95	0.07	157,157,157,157	0
3	TB	A	903	1/1	0.96	0.05	125,125,125,125	0
3	TB	C	903	1/1	0.96	0.07	124,124,124,124	0
3	TB	A	904	1/1	0.96	0.05	122,122,122,122	0
3	TB	B	903	1/1	0.97	0.06	116,116,116,116	0
3	TB	D	902	1/1	0.98	0.05	96,96,96,96	0
3	TB	B	902	1/1	0.99	0.03	80,80,80,80	0
3	TB	A	902	1/1	0.99	0.02	94,94,94,94	0
3	TB	C	902	1/1	0.99	0.04	95,95,95,95	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.

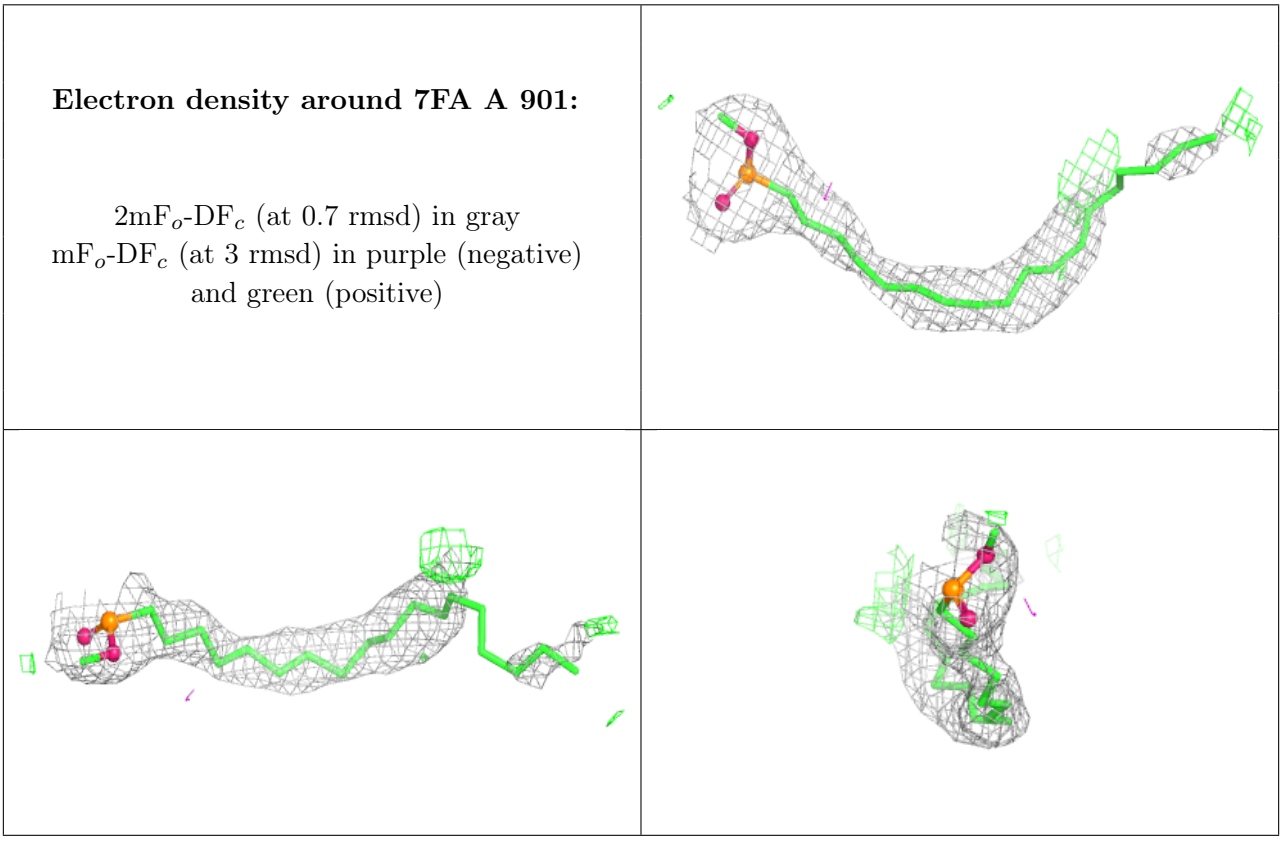
Electron density around 7FA C 901:

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



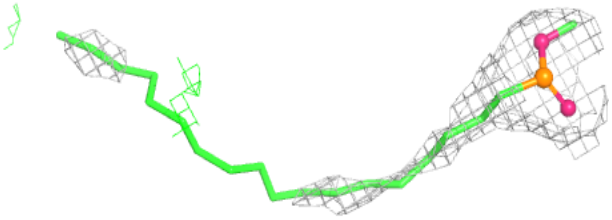
Electron density around 7FA A 901:

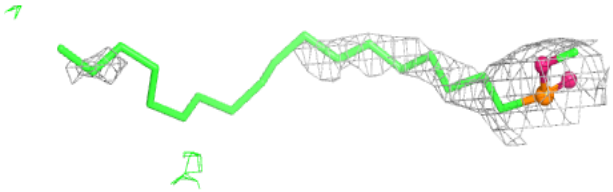
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

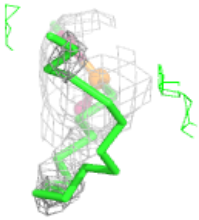


Electron density around 7FA D 901:

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

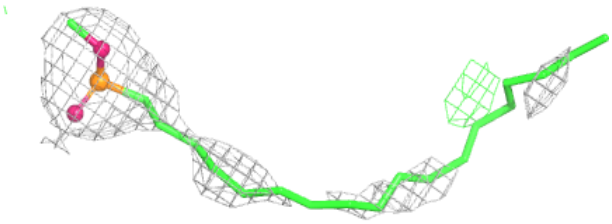


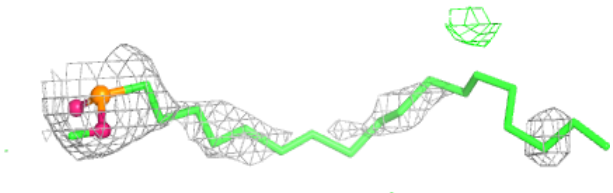


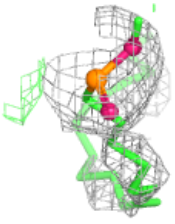


Electron density around 7FA B 901:

$2mF_o$-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 (i)

There are no such residues in this entry.