



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:43 pm BST

PDB ID : 6OHR  
Title : Structure of compound 5 bound human Phospholipase D1 catalytic domain  
Authors : Metrick, C.M.; Chodaparambil, J.V.  
Deposited on : 2019-04-06  
Resolution : 3.20 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](mailto: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

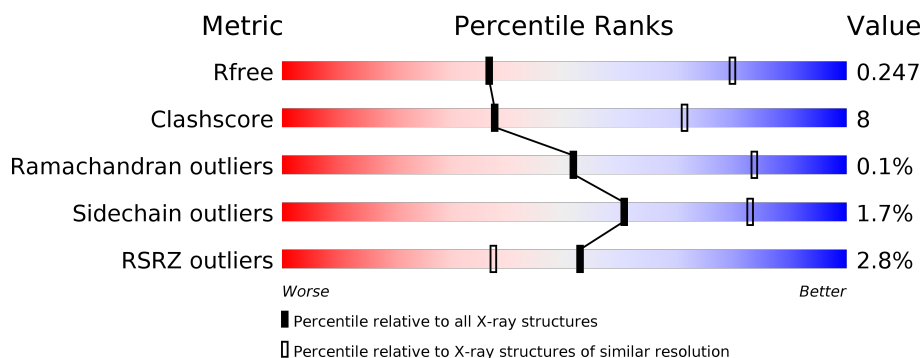
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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	647	<div> <div>71%</div> <div>18%</div> <div>11%</div> </div>
1	B	647	<div> <div>68%</div> <div>19%</div> <div>12%</div> </div>
1	C	647	<div> <div>72%</div> <div>16%</div> <div>12%</div> </div>
1	D	647	<div> <div>70%</div> <div>17%</div> <div>13%</div> </div>
1	E	647	<div> <div>4%</div> <div>71%</div> <div>16%</div> <div>13%</div> </div>
1	F	647	<div> <div>9%</div> <div>69%</div> <div>12%</div> <div>19%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25872 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 Phospholipase D1, chimeric construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4534	2917	783	815	19			
1	B	569	Total	C	N	O	S	0	0	0
			4557	2930	787	821	19			
1	C	572	Total	C	N	O	S	0	0	0
			4503	2904	779	801	19			
1	D	564	Total	C	N	O	S	0	0	0
			4461	2873	771	798	19			
1	E	560	Total	C	N	O	S	0	0	0
			4045	2583	713	735	14			
1	F	526	Total	C	N	O	S	0	0	0
			3580	2266	651	651	12			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLY	-	expression tag	UNP Q13393
A	580	GLY	VAL	linker	UNP Q13393
A	581	SER	LYS	linker	UNP Q13393
A	582	GLY	ARG	linker	UNP Q13393
A	583	SER	VAL	linker	UNP Q13393
A	584	GLY	THR	linker	UNP Q13393
A	587	SER	PRO	linker	UNP Q13393
A	588	GLY	SER	linker	UNP Q13393
A	589	SER	LEU	linker	UNP Q13393
A	592	GLY	LEU	linker	UNP Q13393
A	593	SER	PRO	linker	UNP Q13393
A	594	GLY	ILE	linker	UNP Q13393
A	595	SER	PRO	linker	UNP Q13393
A	597	SER	PRO	linker	UNP Q13393
A	598	GLY	-	linker	UNP Q13393
A	600	HIS	-	linker	UNP Q13393
B	310	GLY	-	expression tag	UNP Q13393

*Continued on next page...*

*Continued from previous page...*

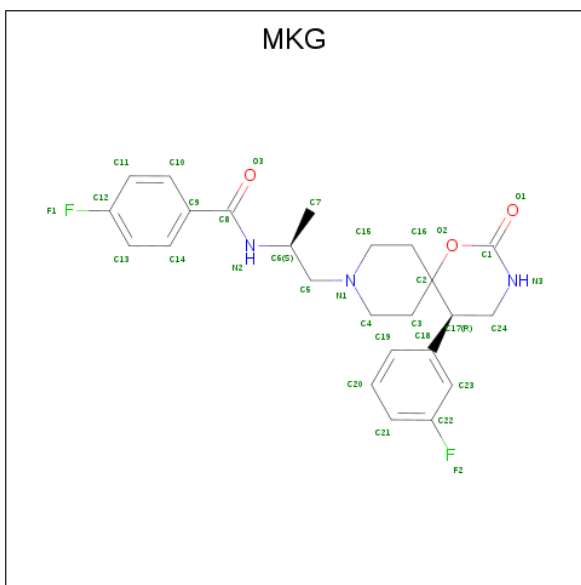
Chain	Residue	Modelled	Actual	Comment	Reference
B	580	GLY	VAL	linker	UNP Q13393
B	581	SER	LYS	linker	UNP Q13393
B	582	GLY	ARG	linker	UNP Q13393
B	583	SER	VAL	linker	UNP Q13393
B	584	GLY	THR	linker	UNP Q13393
B	587	SER	PRO	linker	UNP Q13393
B	588	GLY	SER	linker	UNP Q13393
B	589	SER	LEU	linker	UNP Q13393
B	592	GLY	LEU	linker	UNP Q13393
B	593	SER	PRO	linker	UNP Q13393
B	594	GLY	ILE	linker	UNP Q13393
B	595	SER	PRO	linker	UNP Q13393
B	597	SER	PRO	linker	UNP Q13393
B	598	GLY	-	insertion	UNP Q13393
B	600	HIS	-	linker	UNP Q13393
C	310	GLY	-	expression tag	UNP Q13393
C	580	GLY	VAL	linker	UNP Q13393
C	581	SER	LYS	linker	UNP Q13393
C	582	GLY	ARG	linker	UNP Q13393
C	583	SER	VAL	linker	UNP Q13393
C	584	GLY	THR	linker	UNP Q13393
C	587	SER	PRO	linker	UNP Q13393
C	588	GLY	SER	linker	UNP Q13393
C	589	SER	LEU	linker	UNP Q13393
C	592	GLY	LEU	linker	UNP Q13393
C	593	SER	PRO	linker	UNP Q13393
C	594	GLY	ILE	linker	UNP Q13393
C	595	SER	PRO	linker	UNP Q13393
C	597	SER	PRO	linker	UNP Q13393
C	598	GLY	-	insertion	UNP Q13393
C	600	HIS	-	linker	UNP Q13393
D	310	GLY	-	expression tag	UNP Q13393
D	580	GLY	VAL	linker	UNP Q13393
D	581	SER	LYS	linker	UNP Q13393
D	582	GLY	ARG	linker	UNP Q13393
D	583	SER	VAL	linker	UNP Q13393
D	584	GLY	THR	linker	UNP Q13393
D	587	SER	PRO	linker	UNP Q13393
D	588	GLY	SER	linker	UNP Q13393
D	589	SER	LEU	linker	UNP Q13393
D	592	GLY	LEU	linker	UNP Q13393
D	593	SER	PRO	linker	UNP Q13393

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	594	GLY	ILE	linker	UNP Q13393
D	595	SER	PRO	linker	UNP Q13393
D	597	SER	PRO	linker	UNP Q13393
D	598	GLY	-	insertion	UNP Q13393
D	600	HIS	-	linker	UNP Q13393
E	310	GLY	-	expression tag	UNP Q13393
E	580	GLY	VAL	linker	UNP Q13393
E	581	SER	LYS	linker	UNP Q13393
E	582	GLY	ARG	linker	UNP Q13393
E	583	SER	VAL	linker	UNP Q13393
E	584	GLY	THR	linker	UNP Q13393
E	587	SER	PRO	linker	UNP Q13393
E	588	GLY	SER	linker	UNP Q13393
E	589	SER	LEU	linker	UNP Q13393
E	592	GLY	LEU	linker	UNP Q13393
E	593	SER	PRO	linker	UNP Q13393
E	594	GLY	ILE	linker	UNP Q13393
E	595	SER	PRO	linker	UNP Q13393
E	597	SER	PRO	linker	UNP Q13393
E	598	GLY	-	insertion	UNP Q13393
E	600	HIS	-	linker	UNP Q13393
F	310	GLY	-	expression tag	UNP Q13393
F	580	GLY	VAL	linker	UNP Q13393
F	581	SER	LYS	linker	UNP Q13393
F	582	GLY	ARG	linker	UNP Q13393
F	583	SER	VAL	linker	UNP Q13393
F	584	GLY	THR	linker	UNP Q13393
F	587	SER	PRO	linker	UNP Q13393
F	588	GLY	SER	linker	UNP Q13393
F	589	SER	LEU	linker	UNP Q13393
F	592	GLY	LEU	linker	UNP Q13393
F	593	SER	PRO	linker	UNP Q13393
F	594	GLY	ILE	linker	UNP Q13393
F	595	SER	PRO	linker	UNP Q13393
F	597	SER	PRO	linker	UNP Q13393
F	598	GLY	-	linker	UNP Q13393
F	600	HIS	-	linker	UNP Q13393

- Molecule 2 is 4-fluoro-N-{(2S)-1-[(5R)-5-(3-fluorophenyl)-2-oxo-1-oxa-3,9-diazaspiro[5.5]undecan-9-yl]propan-2-yl}benzamide (three-letter code: MKG) (formula: C<sub>24</sub>H<sub>27</sub>F<sub>2</sub>N<sub>3</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by author).

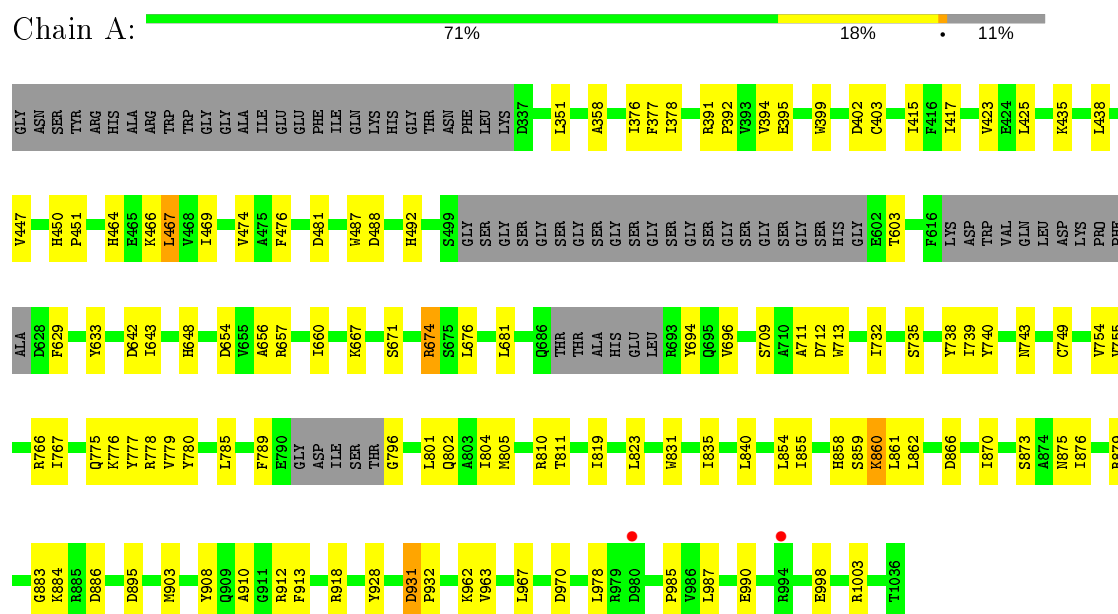


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 32	C 24	F 2	N 3	O 3	0	0
2	B	1	Total 32	C 24	F 2	N 3	O 3	0	0
2	C	1	Total 32	C 24	F 2	N 3	O 3	0	0
2	D	1	Total 32	C 24	F 2	N 3	O 3	0	0
2	E	1	Total 32	C 24	F 2	N 3	O 3	0	0
2	F	1	Total 32	C 24	F 2	N 3	O 3	0	0

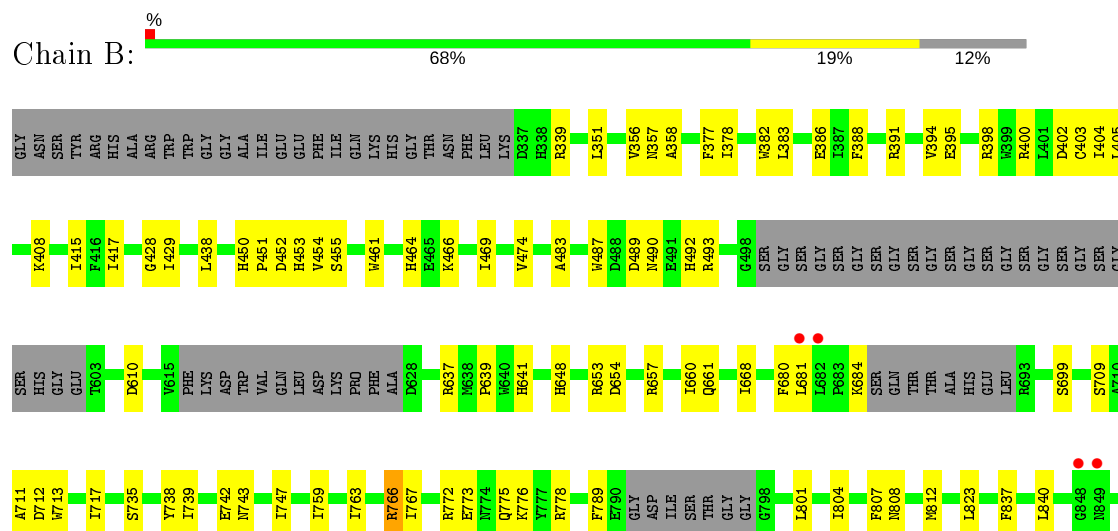
### 3 Residue-property plots

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: Phospholipase D1, chimeric construct



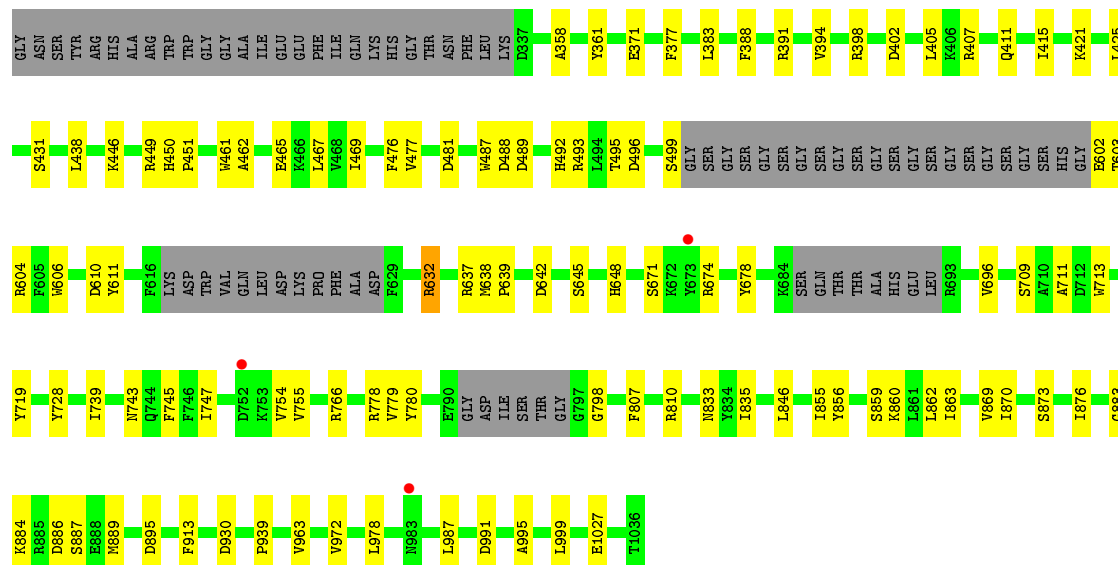
- Molecule 1: Phospholipase D1, chimeric construct





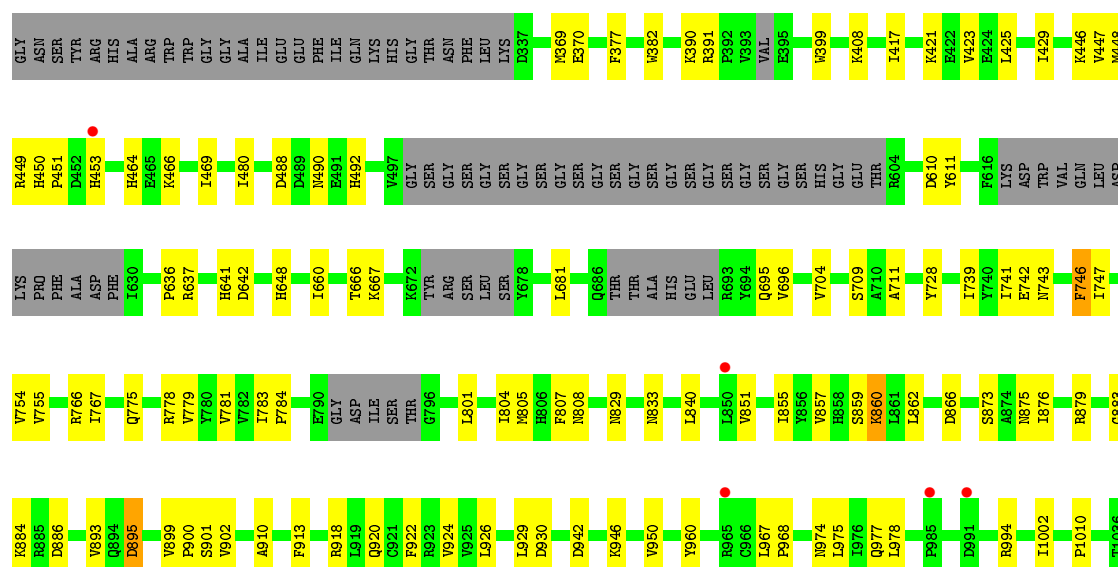
- Molecule 1: Phospholipase D1, chimeric construct

Chain C: 72% 16% 12%



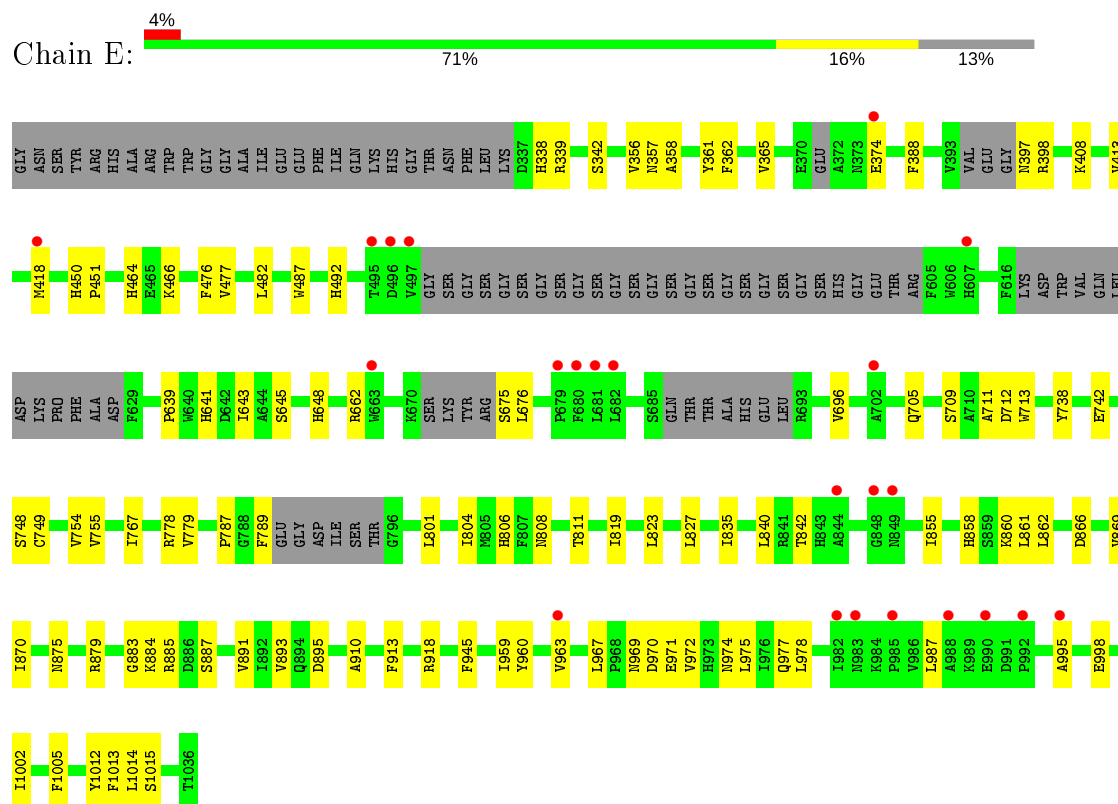
- Molecule 1: Phospholipase D1, chimeric construct

Chain D: 70% 17% 13%

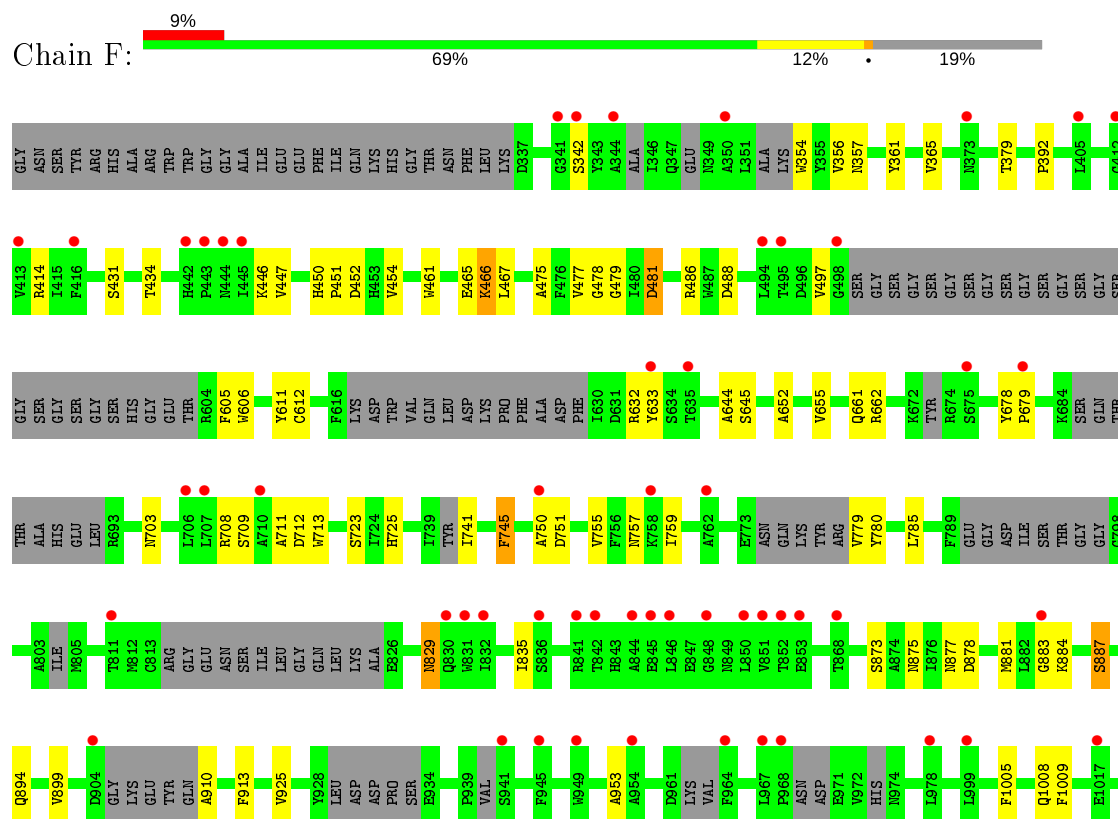


- Molecule 1: Phospholipase D1, chimeric construct





- Molecule 1: Phospholipase D1, chimeric construct





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.04Å 155.11Å 273.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 3.20 48.36 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.36-3.20) 99.9 (48.36-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.14_3211: ???)	Depositor
R, $R_{free}$	0.221 , 0.247 0.221 , 0.247	Depositor DCC
$R_{free}$ test set	6614 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.0	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	25872	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MKG

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	0.25	0/4649	0.46	0/6325
1	B	0.25	0/4671	0.45	0/6341
1	C	0.25	0/4617	0.45	0/6279
1	D	0.25	0/4573	0.44	0/6214
1	E	0.25	0/4148	0.45	0/5677
1	F	0.24	0/3653	0.43	0/4994
All	All	0.25	0/26311	0.45	0/35830

There are no bond length outliers.

There are no bond angle outliers.

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	4534	0	4277	74	0
1	B	4557	0	4361	79	0
1	C	4503	0	4254	54	3
1	D	4461	0	4218	66	0
1	E	4045	0	3405	65	0
1	F	3580	0	2781	46	0
2	A	32	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	32	0	0	1	3
2	C	32	0	0	0	0
2	D	32	0	0	1	0
2	E	32	0	0	0	0
2	F	32	0	0	0	0
All	All	25872	0	23296	380	3

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 8.

All (380) 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:394:VAL:HG23	1:A:395:GLU:H	1.30	0.96
1:D:377:PHE:HB2	1:D:469:ILE:HB	1.57	0.85
1:A:654:ASP:OD1	1:A:657:ARG:NH1	2.21	0.74
1:A:394:VAL:HG23	1:A:395:GLU:N	2.02	0.73
1:A:779:VAL:HB	1:A:835:ILE:HG13	1.70	0.73
1:A:860:LYS:NZ	1:A:875:ASN:OD1	2.20	0.73
1:B:735:SER:O	1:B:766:ARG:NH1	2.21	0.73
1:B:840:LEU:HD12	1:B:1005:PHE:HB2	1.72	0.71
1:B:776:LYS:NZ	1:B:904:ASP:OD1	2.23	0.71
1:A:862:LEU:HD23	1:A:870:ILE:HD12	1.72	0.71
1:C:972:VAL:HG11	1:C:978:LEU:HD12	1.73	0.70
1:E:789:PHE:HB2	1:E:801:LEU:HD23	1.72	0.69
1:D:866:ASP:OD2	1:D:918:ARG:NH2	2.22	0.69
1:D:974:ASN:HB3	1:D:977:GLN:HG3	1.73	0.69
1:B:357:ASN:ND2	1:B:490:ASN:OD1	2.26	0.69
1:B:899:VAL:HG23	1:B:912:ARG:HG2	1.74	0.69
1:C:377:PHE:HB2	1:C:469:ILE:HB	1.76	0.68
1:A:912:ARG:NH2	1:D:695:GLN:O	2.27	0.68
1:B:395:GLU:OE1	1:B:398:ARG:NH1	2.26	0.67
1:D:766:ARG:NH2	1:D:775:GLN:OE1	2.27	0.67
1:F:741:ILE:N	1:F:780:TYR:O	2.28	0.67
1:E:450:HIS:CD2	1:E:451:PRO:HA	2.31	0.66
1:D:840:LEU:HB3	1:D:855:ILE:HB	1.77	0.66
1:F:661:GLN:OE1	1:F:708:ARG:NH1	2.23	0.66
1:C:863:ILE:HG12	1:C:869:VAL:HG22	1.77	0.65
1:B:641:HIS:NE2	1:B:742:GLU:OE2	2.29	0.65
1:E:641:HIS:NE2	1:E:742:GLU:OE2	2.27	0.65
1:E:339:ARG:HB3	1:E:705:GLN:HE22	1.61	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:VAL:HG12	1:B:395:GLU:HG3	1.78	0.65
1:F:709:SER:HB3	1:F:883:GLY:HA2	1.79	0.65
1:C:711:ALA:HB2	1:C:884:LYS:HA	1.78	0.63
1:C:779:VAL:HB	1:C:835:ILE:HG13	1.81	0.63
1:A:840:LEU:HB3	1:A:855:ILE:HB	1.82	0.62
1:F:465:GLU:OE1	1:F:887:SER:OG	2.19	0.60
1:B:943:LYS:O	1:B:947:GLU:HB2	2.01	0.60
1:D:423:VAL:HG12	1:D:425:LEU:H	1.67	0.60
1:D:741:ILE:HD11	1:D:781:VAL:HG13	1.83	0.60
1:E:974:ASN:HB3	1:E:977:GLN:HG3	1.84	0.60
1:A:732:ILE:HG12	1:A:739:ILE:HD13	1.83	0.60
1:A:464:HIS:O	1:A:466:LYS:NZ	2.31	0.59
1:C:963:VAL:HA	1:C:987:LEU:HD23	1.84	0.59
1:A:667:LYS:HG3	1:A:676:LEU:HD12	1.84	0.58
1:C:488:ASP:OD2	1:C:492:HIS:ND1	2.35	0.58
1:C:388:PHE:O	1:C:391:ARG:NH2	2.36	0.58
1:A:656:ALA:O	1:A:660:ILE:HG12	2.04	0.58
1:C:709:SER:HB3	1:C:883:GLY:HA2	1.85	0.58
1:E:711:ALA:HB2	1:E:884:LYS:HA	1.84	0.58
1:B:654:ASP:OD1	1:B:657:ARG:NH1	2.31	0.58
1:C:778:ARG:NH1	1:C:833:ASN:O	2.36	0.58
1:A:435:LYS:NZ	1:A:447:VAL:O	2.36	0.58
1:D:739:ILE:HG22	1:D:779:VAL:HG13	1.84	0.58
1:E:477:VAL:HG21	1:E:891:VAL:HG21	1.85	0.57
1:C:361:TYR:HE1	1:C:476:PHE:HB3	1.69	0.57
1:C:431:SER:HB2	1:C:449:ARG:HH11	1.70	0.57
1:B:711:ALA:HB2	1:B:884:LYS:HA	1.86	0.56
1:E:709:SER:HB3	1:E:883:GLY:HA2	1.87	0.56
1:B:377:PHE:HB2	1:B:469:ILE:HB	1.88	0.56
1:B:919:LEU:O	1:B:923:ARG:HG3	2.05	0.56
1:C:489:ASP:OD2	1:C:493:ARG:NH2	2.39	0.56
1:F:875:ASN:HB2	1:F:877:ASN:ND2	2.20	0.56
1:B:963:VAL:HG12	1:B:988:ALA:HB2	1.87	0.56
1:B:747:ILE:HG23	1:B:807:PHE:HB3	1.88	0.56
1:A:417:ILE:HD13	1:A:438:LEU:HD13	1.88	0.56
1:B:653:ARG:HH11	1:B:684:LYS:C	2.09	0.56
1:D:641:HIS:NE2	1:D:742:GLU:OE2	2.38	0.55
1:A:928:TYR:HE2	1:A:1003:ARG:HH22	1.55	0.55
1:A:962:LYS:NZ	1:A:998:GLU:OE2	2.39	0.55
1:A:709:SER:HB3	1:A:883:GLY:HA2	1.90	0.54
1:B:358:ALA:HB3	1:B:487:TRP:HA	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:446:LYS:HB3	1:F:678:TYR:CE2	2.42	0.54
1:D:709:SER:HB3	1:D:883:GLY:HA2	1.88	0.54
1:B:900:PRO:HG2	1:C:371:GLU:HG2	1.89	0.54
1:C:739:ILE:HG13	1:C:779:VAL:HG13	1.88	0.54
1:F:759:ILE:HD11	1:F:881:MET:HG3	1.88	0.54
1:B:739:ILE:HG13	1:B:862:LEU:HD11	1.89	0.54
1:F:466:LYS:NZ	1:F:481:ASP:OD2	2.41	0.54
1:F:461:TRP:HB2	1:F:713:TRP:CZ2	2.43	0.53
1:B:840:LEU:HB3	1:B:855:ILE:HB	1.88	0.53
1:B:668:ILE:HD11	1:B:680:PHE:HZ	1.74	0.53
1:B:840:LEU:HD11	1:B:925:VAL:HG12	1.90	0.53
1:E:840:LEU:HB3	1:E:855:ILE:HB	1.89	0.53
1:F:379:THR:HG22	1:F:467:LEU:HG	1.89	0.53
1:E:860:LYS:HE2	1:E:875:ASN:OD1	2.08	0.53
1:A:796:GLY:O	1:A:802:GLN:NE2	2.42	0.53
1:F:711:ALA:HB2	1:F:884:LYS:HA	1.91	0.53
1:D:754:VAL:HG23	1:D:755:VAL:HG23	1.91	0.53
1:F:703:ASN:N	1:F:894:GLN:O	2.38	0.53
1:B:464:HIS:O	1:B:466:LYS:NZ	2.39	0.53
1:A:970:ASP:N	1:A:970:ASP:OD1	2.42	0.52
1:D:778:ARG:NH1	1:D:833:ASN:O	2.43	0.52
1:D:974:ASN:OD1	1:D:975:LEU:N	2.42	0.52
1:F:745:PHE:HE1	1:F:877:ASN:ND2	2.06	0.52
1:A:754:VAL:HG23	1:A:755:VAL:HG23	1.92	0.52
1:B:840:LEU:HD23	1:B:857:VAL:HG22	1.90	0.52
1:D:747:ILE:HG23	1:D:807:PHE:HB3	1.89	0.52
1:B:709:SER:HB3	1:B:883:GLY:HA2	1.91	0.52
1:A:474:VAL:HG21	1:A:694:TYR:HD2	1.74	0.52
1:B:899:VAL:CG2	1:B:912:ARG:HG2	2.38	0.52
1:B:933:SER:O	1:B:937:GLN:NE2	2.28	0.52
1:F:606:TRP:O	1:F:632:ARG:NH2	2.38	0.52
1:A:394:VAL:CG2	1:A:395:GLU:H	2.13	0.52
1:B:660:ILE:HG12	1:B:681:LEU:HB3	1.91	0.52
1:C:860:LYS:HD3	1:C:873:SER:HA	1.91	0.52
1:C:709:SER:O	1:C:887:SER:HA	2.09	0.52
1:B:453:HIS:ND1	1:B:454:VAL:HG13	2.23	0.52
1:C:358:ALA:HB3	1:C:487:TRP:HA	1.92	0.52
1:A:735:SER:HG	1:A:777:TYR:HH	1.43	0.52
1:F:431:SER:HA	1:F:434:THR:HG22	1.91	0.52
1:A:648:HIS:CE1	1:A:696:VAL:HG22	2.44	0.51
1:C:446:LYS:HD3	1:C:678:TYR:CD1	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:374:GLU:O	1:E:413:VAL:HG23	2.10	0.51
1:B:934:GLU:OE1	1:B:934:GLU:N	2.42	0.51
1:E:970:ASP:HB3	1:E:1012:TYR:H	1.75	0.51
1:E:356:VAL:HA	1:E:643:ILE:HD13	1.93	0.51
1:E:858:HIS:O	1:E:860:LYS:HE3	2.11	0.51
1:E:869:VAL:HG13	1:E:893:VAL:HB	1.93	0.51
1:D:875:ASN:ND2	2:D:1101:MKG:O1	2.42	0.51
1:D:784:PRO:HD3	1:D:857:VAL:HB	1.92	0.51
1:E:712:ASP:OD1	1:E:713:TRP:N	2.44	0.51
1:E:767:ILE:HG21	1:E:823:LEU:HD21	1.93	0.51
1:D:866:ASP:HB3	1:D:910:ALA:HB1	1.93	0.50
1:A:776:LYS:HD3	1:A:778:ARG:HH21	1.74	0.50
1:A:643:ILE:HG21	1:A:861:LEU:HD13	1.92	0.50
1:F:466:LYS:HD2	1:F:479:GLY:C	2.31	0.50
1:B:789:PHE:HB2	1:B:801:LEU:HG	1.91	0.50
1:A:467:LEU:HA	1:A:476:PHE:O	2.12	0.50
1:A:743:ASN:ND2	1:A:876:ILE:HG13	2.26	0.50
1:D:464:HIS:O	1:D:466:LYS:NZ	2.33	0.50
1:E:464:HIS:O	1:E:466:LYS:NZ	2.32	0.50
1:E:972:VAL:HG11	1:E:978:LEU:HD12	1.93	0.50
1:F:750:ALA:HA	1:F:755:VAL:HG23	1.94	0.50
1:B:743:ASN:HA	1:B:859:SER:O	2.12	0.49
1:C:391:ARG:NH1	1:C:610:ASP:OD2	2.45	0.49
1:E:779:VAL:HB	1:E:835:ILE:HG13	1.92	0.49
1:A:392:PRO:HB3	1:A:603:THR:HG21	1.94	0.49
1:D:918:ARG:HD3	1:D:922:PHE:CE2	2.47	0.49
1:F:392:PRO:HG3	1:F:605:PHE:CE1	2.46	0.49
1:A:738:TYR:OH	1:A:866:ASP:OD1	2.20	0.49
1:E:754:VAL:HG23	1:E:755:VAL:HG23	1.93	0.49
1:D:767:ILE:HD11	1:D:779:VAL:HG21	1.93	0.49
1:D:450:HIS:CD2	1:D:451:PRO:HA	2.48	0.49
1:E:361:TYR:HE1	1:E:476:PHE:HB3	1.77	0.49
1:A:732:ILE:HA	1:A:739:ILE:HD11	1.94	0.49
1:E:388:PHE:HE1	1:E:397:ASN:HA	1.78	0.49
1:E:362:PHE:HE1	1:E:482:LEU:HD23	1.77	0.49
1:E:804:ILE:O	1:E:808:ASN:ND2	2.46	0.49
1:F:447:VAL:O	1:F:678:TYR:OH	2.20	0.49
1:F:611:TYR:CE1	1:F:632:ARG:HA	2.48	0.49
1:D:899:VAL:N	1:D:910:ALA:O	2.37	0.48
1:D:711:ALA:HB2	1:D:884:LYS:HA	1.94	0.48
1:C:495:THR:HG22	1:C:846:LEU:HB2	1.94	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LEU:HD12	1:B:699:SER:HB2	1.95	0.48
1:B:804:ILE:O	1:B:808:ASN:ND2	2.46	0.48
1:C:405:LEU:HD22	1:C:415:ILE:HD13	1.94	0.48
1:D:382:TRP:CD1	1:D:429:ILE:HG23	2.49	0.48
1:C:862:LEU:HD23	1:C:870:ILE:HD12	1.95	0.48
1:A:660:ILE:HD12	1:A:681:LEU:HB3	1.96	0.48
1:D:895:ASP:OD2	1:D:913:PHE:N	2.44	0.48
1:E:895:ASP:OD1	1:E:913:PHE:HB3	2.13	0.48
1:F:475:ALA:HB1	1:F:655:VAL:HG21	1.94	0.48
1:B:661:GLN:NE2	1:B:717:ILE:HD11	2.29	0.48
1:C:467:LEU:HD11	1:C:889:MET:HG3	1.95	0.48
1:D:739:ILE:CG2	1:D:779:VAL:HG13	2.44	0.48
1:E:356:VAL:HG12	1:E:357:ASN:ND2	2.29	0.48
1:B:778:ARG:HD2	1:B:945:PHE:CD1	2.48	0.48
1:D:488:ASP:OD2	1:D:492:HIS:ND1	2.46	0.48
1:E:408:LYS:O	1:E:413:VAL:HG12	2.13	0.48
1:A:351:LEU:HB2	1:A:648:HIS:HB2	1.96	0.48
1:B:489:ASP:OD2	1:B:493:ARG:NH2	2.47	0.47
1:A:963:VAL:HA	1:A:987:LEU:HD12	1.96	0.47
1:B:773:GLU:OE1	1:B:775:GLN:NE2	2.47	0.47
1:E:365:VAL:HG22	1:E:476:PHE:CD2	2.50	0.47
1:F:745:PHE:HE1	1:F:877:ASN:HD22	1.62	0.47
1:D:860:LYS:HD3	1:D:873:SER:HA	1.96	0.47
1:E:787:PRO:HB2	1:E:801:LEU:HD22	1.96	0.47
1:E:970:ASP:OD1	1:E:970:ASP:N	2.48	0.47
1:F:751:ASP:H	1:F:755:VAL:HG23	1.79	0.47
1:F:452:ASP:OD1	1:F:454:VAL:HG22	2.15	0.47
1:A:488:ASP:OD2	1:A:492:HIS:ND1	2.47	0.47
1:C:606:TRP:O	1:C:632:ARG:NH1	2.32	0.47
1:C:496:ASP:O	1:C:632:ARG:HD2	2.15	0.47
1:D:960:TYR:CZ	1:D:1002:ILE:HD13	2.49	0.47
1:F:478:GLY:HA3	1:F:644:ALA:HA	1.95	0.47
1:F:779:VAL:HG22	1:F:835:ILE:HA	1.97	0.47
1:C:637:ARG:NH2	1:C:639:PRO:HA	2.30	0.47
1:D:391:ARG:NH2	1:D:610:ASP:OD2	2.48	0.47
1:E:970:ASP:HB2	1:E:1012:TYR:HB2	1.95	0.47
1:A:394:VAL:CG2	1:A:399:TRP:HD1	2.28	0.47
1:D:480:ILE:HG12	1:D:642:ASP:HB3	1.96	0.47
1:A:660:ILE:HG23	1:A:681:LEU:HB2	1.96	0.47
1:C:754:VAL:HG23	1:C:755:VAL:HG23	1.97	0.46
1:E:879:ARG:O	1:E:885:ARG:HB2	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:ILE:O	1:D:808:ASN:ND2	2.46	0.46
1:D:450:HIS:CG	1:D:451:PRO:HA	2.51	0.46
1:A:738:TYR:OH	1:A:918:ARG:HD3	2.16	0.46
1:E:858:HIS:ND1	1:E:858:HIS:O	2.48	0.46
1:B:391:ARG:NH2	1:B:610:ASP:OD2	2.49	0.46
1:B:963:VAL:HG13	1:B:995:ALA:HB1	1.97	0.46
1:D:660:ILE:HG23	1:D:681:LEU:HB2	1.98	0.46
1:C:611:TYR:CE2	1:C:637:ARG:HB3	2.51	0.46
1:C:995:ALA:O	1:C:999:LEU:HG	2.16	0.46
1:E:675:SER:OG	1:E:676:LEU:N	2.47	0.46
1:B:402:ASP:OD1	1:B:403:CYS:N	2.49	0.46
1:A:931:ASP:CG	1:A:932:PRO:HD2	2.37	0.46
1:B:974:ASN:HB2	1:B:977:GLN:HG3	1.97	0.46
1:D:946:LYS:HA	1:D:950:VAL:HG22	1.98	0.46
1:E:643:ILE:HG13	1:E:861:LEU:HD23	1.98	0.46
1:B:386:GLU:HG2	1:B:402:ASP:OD2	2.16	0.45
1:C:648:HIS:CE1	1:C:696:VAL:HG22	2.51	0.45
1:E:823:LEU:HB3	1:E:827:LEU:HD11	1.97	0.45
1:E:709:SER:O	1:E:887:SER:HA	2.16	0.45
1:F:785:LEU:HA	1:F:1009:PHE:HE1	1.82	0.45
1:F:953:ALA:HB1	1:F:1008:GLN:N	2.30	0.45
1:A:735:SER:OG	1:A:777:TYR:OH	2.24	0.45
1:A:967:LEU:HD13	1:A:978:LEU:HD11	1.99	0.45
1:E:987:LEU:HD22	1:E:995:ALA:HB2	1.98	0.45
1:A:392:PRO:O	1:A:394:VAL:HG13	2.17	0.45
1:D:611:TYR:CE2	1:D:637:ARG:HB3	2.51	0.45
1:B:661:GLN:HE22	1:B:717:ILE:HD11	1.80	0.45
1:C:407:ARG:O	1:C:411:GLN:HG3	2.17	0.45
1:E:742:GLU:HB3	1:E:861:LEU:HG	1.97	0.45
1:A:402:ASP:OD1	1:A:403:CYS:N	2.50	0.45
1:E:748:SER:OG	1:E:749:CYS:N	2.47	0.45
1:A:712:ASP:OD1	1:A:713:TRP:N	2.50	0.45
1:C:462:ALA:N	1:C:886:ASP:OD1	2.28	0.45
1:D:968:PRO:HB2	1:D:1010:PRO:HG3	1.98	0.45
1:D:739:ILE:HG13	1:D:862:LEU:HD11	1.98	0.45
1:D:667:LYS:HE2	1:D:667:LYS:HB3	1.72	0.45
1:E:862:LEU:O	1:E:869:VAL:HA	2.17	0.45
1:E:974:ASN:OD1	1:E:975:LEU:N	2.50	0.45
1:F:497:VAL:HG23	1:F:633:TYR:CD1	2.52	0.45
1:D:746:PHE:HB2	1:D:783:ILE:CD1	2.47	0.44
1:D:636:PRO:HG3	1:D:851:VAL:HB	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:922:PHE:O	1:D:926:LEU:HB2	2.17	0.44
1:A:358:ALA:HB3	1:A:487:TRP:HA	1.99	0.44
1:A:858:HIS:O	1:A:858:HIS:ND1	2.50	0.44
1:C:461:TRP:HB2	1:C:713:TRP:CZ2	2.52	0.44
1:E:870:ILE:HA	1:E:891:VAL:O	2.17	0.44
1:A:378:ILE:HB	1:A:417:ILE:HG12	1.99	0.44
1:A:860:LYS:HD3	1:A:873:SER:HA	1.99	0.44
1:B:405:LEU:HD22	1:B:415:ILE:HG21	1.99	0.44
1:B:778:ARG:HG3	1:B:940:VAL:HA	1.98	0.44
1:C:450:HIS:CG	1:C:451:PRO:HA	2.52	0.44
1:D:370:GLU:O	1:D:408:LYS:NZ	2.39	0.44
1:F:361:TYR:O	1:F:365:VAL:HG23	2.17	0.44
1:B:877:ASN:HB2	1:B:1036:THR:O	2.17	0.44
1:B:637:ARG:NH2	1:B:639:PRO:HA	2.32	0.44
1:D:390:LYS:HD2	1:D:399:TRP:CD2	2.53	0.44
1:E:1013:PHE:CE2	1:E:1014:LEU:HG	2.53	0.44
1:A:866:ASP:HB3	1:A:910:ALA:HB1	1.99	0.44
1:B:382:TRP:CD1	1:B:429:ILE:HG23	2.52	0.44
1:B:388:PHE:HB2	1:B:391:ARG:HE	1.82	0.44
1:B:400:ARG:O	1:B:404:ILE:HG13	2.17	0.44
1:F:925:VAL:O	1:F:1005:PHE:N	2.39	0.44
1:A:376:ILE:HB	1:A:415:ILE:HG12	2.00	0.44
1:C:642:ASP:HA	1:C:859:SER:HB3	2.00	0.44
1:C:446:LYS:HD3	1:C:678:TYR:HD1	1.81	0.44
1:E:960:TYR:CZ	1:E:1002:ILE:HD13	2.53	0.44
1:D:967:LEU:HD13	1:D:978:LEU:HD11	2.00	0.44
1:E:963:VAL:HG13	1:E:995:ALA:HB1	2.00	0.44
1:F:481:ASP:O	1:F:486:ARG:HG3	2.18	0.44
1:A:711:ALA:HB2	1:A:884:LYS:HA	1.99	0.43
1:B:712:ASP:OD1	1:B:713:TRP:N	2.51	0.43
1:B:858:HIS:O	1:B:858:HIS:ND1	2.50	0.43
1:D:743:ASN:ND2	1:D:876:ILE:HG13	2.33	0.43
1:D:746:PHE:HB2	1:D:783:ILE:HD13	1.99	0.43
1:D:746:PHE:O	1:D:808:ASN:HA	2.18	0.43
1:A:377:PHE:HB2	1:A:469:ILE:HB	2.01	0.43
1:A:766:ARG:NH2	1:A:775:GLN:OE1	2.51	0.43
1:C:383:LEU:HD22	1:C:438:LEU:HD11	2.01	0.43
1:C:492:HIS:CD2	1:C:855:ILE:HD13	2.54	0.43
1:F:652:ALA:O	1:F:655:VAL:HG22	2.17	0.43
1:B:461:TRP:HB2	1:B:713:TRP:CZ2	2.54	0.43
1:C:496:ASP:OD2	1:C:604:ARG:HG3	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:747:ILE:HG23	1:C:807:PHE:HB3	2.00	0.43
1:B:356:VAL:HG12	1:B:357:ASN:ND2	2.34	0.43
1:B:378:ILE:HB	1:B:417:ILE:HG12	2.00	0.43
1:C:638:MET:SD	1:C:856:TYR:HB2	2.59	0.43
1:A:785:LEU:HB2	1:A:854:LEU:HD22	2.01	0.43
1:B:383:LEU:HD22	1:B:438:LEU:HD11	2.00	0.43
1:B:339:ARG:NH1	1:B:894:GLN:OE1	2.51	0.43
1:C:743:ASN:HA	1:C:859:SER:O	2.18	0.43
1:D:899:VAL:HG22	1:D:900:PRO:HD2	2.00	0.43
1:D:920:GLN:O	1:D:924:VAL:HG23	2.18	0.43
1:B:767:ILE:HG21	1:B:823:LEU:HD21	2.01	0.43
1:B:812:MET:HG3	1:B:837:PHE:CZ	2.53	0.43
1:E:492:HIS:CD2	1:E:855:ILE:HD13	2.54	0.43
1:B:860:LYS:HG3	1:B:873:SER:HA	2.01	0.43
1:D:417:ILE:O	1:D:447:VAL:HA	2.19	0.43
1:D:743:ASN:HA	1:D:859:SER:O	2.18	0.43
1:E:738:TYR:OH	1:E:918:ARG:HD3	2.19	0.43
1:F:354:TRP:HB3	1:F:913:PHE:CZ	2.53	0.43
1:A:671:SER:HA	1:A:674:ARG:O	2.19	0.43
1:C:465:GLU:HB2	1:C:889:MET:HB2	2.01	0.43
1:F:829:ASN:O	1:F:829:ASN:ND2	2.44	0.43
1:C:743:ASN:ND2	1:C:876:ILE:HG13	2.34	0.43
1:C:402:ASP:OD2	1:D:829:ASN:ND2	2.47	0.42
1:D:879:ARG:HD3	1:D:886:ASP:OD2	2.19	0.42
1:E:477:VAL:O	1:E:645:SER:N	2.47	0.42
1:F:342:SER:HA	1:F:723:SER:OG	2.19	0.42
1:B:492:HIS:CD2	1:B:855:ILE:HD13	2.53	0.42
1:D:648:HIS:NE2	1:D:696:VAL:HG22	2.34	0.42
1:A:743:ASN:HA	1:A:859:SER:O	2.19	0.42
1:A:767:ILE:HD11	1:A:779:VAL:HG21	2.00	0.42
1:B:452:ASP:HB3	1:B:455:SER:HB2	1.99	0.42
1:D:901:SER:OG	1:D:902:VAL:N	2.52	0.42
1:C:602:GLU:HB3	1:C:603:THR:H	1.55	0.42
1:D:449:ARG:HH22	1:D:453:HIS:HE1	1.67	0.42
1:A:450:HIS:CG	1:A:451:PRO:HA	2.55	0.42
1:D:448:MET:HE3	1:D:666:THR:HB	2.01	0.42
1:E:842:THR:HB	1:E:1005:PHE:HD1	1.84	0.42
1:E:639:PRO:HB2	1:E:855:ILE:HG23	2.02	0.42
1:F:899:VAL:N	1:F:910:ALA:O	2.39	0.42
1:D:421:LYS:HB2	1:D:449:ARG:HB3	2.02	0.42
1:A:879:ARG:O	1:A:886:ASP:HB2	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:PRO:HB3	1:A:990:GLU:OE2	2.19	0.42
1:A:875:ASN:ND2	2:A:1101:MKG:O1	2.50	0.42
1:B:776:LYS:HD2	1:B:778:ARG:NH2	2.35	0.42
1:B:492:HIS:HD2	1:B:855:ILE:HD13	1.84	0.42
1:D:704:VAL:HG22	1:D:893:VAL:HG22	2.01	0.42
1:A:823:LEU:HD23	1:A:831:TRP:HB2	2.01	0.42
1:E:1012:TYR:O	1:E:1015:SER:OG	2.37	0.42
1:F:478:GLY:O	1:F:873:SER:HB3	2.19	0.42
1:F:712:ASP:N	1:F:712:ASP:OD1	2.53	0.42
1:A:789:PHE:HE2	1:A:804:ILE:HD12	1.85	0.42
1:B:400:ARG:HD3	1:B:402:ASP:OD1	2.20	0.42
1:D:942:ASP:OD1	1:D:942:ASP:N	2.53	0.42
1:E:643:ILE:HG13	1:E:861:LEU:CD2	2.50	0.42
1:E:866:ASP:HB3	1:E:910:ALA:HB1	2.02	0.42
1:F:446:LYS:HB3	1:F:678:TYR:HE2	1.85	0.42
1:D:490:ASN:HB3	1:D:929:LEU:HD21	2.01	0.41
1:E:358:ALA:HB3	1:E:487:TRP:HA	2.01	0.41
1:E:967:LEU:HD22	1:E:1013:PHE:HE1	1.84	0.41
1:F:450:HIS:CG	1:F:451:PRO:HA	2.55	0.41
1:F:755:VAL:HG12	1:F:1036:THR:HG23	2.02	0.41
1:A:801:LEU:HD23	1:A:805:MET:HG3	2.03	0.41
1:A:858:HIS:CE1	1:A:860:LYS:HE2	2.55	0.41
1:C:987:LEU:HD12	1:C:991:ASP:HB2	2.01	0.41
1:E:778:ARG:HD2	1:E:945:PHE:CG	2.55	0.41
1:C:895:ASP:OD2	1:C:913:PHE:N	2.52	0.41
1:A:811:THR:O	1:A:819:ILE:HG13	2.20	0.41
1:A:903:MET:HE1	1:A:908:TYR:CE2	2.55	0.41
1:B:862:LEU:HD23	1:B:870:ILE:HD12	2.02	0.41
1:D:369:MET:O	1:D:408:LYS:HE2	2.21	0.41
1:F:477:VAL:O	1:F:645:SER:N	2.51	0.41
1:B:709:SER:O	1:B:887:SER:HA	2.20	0.41
1:E:648:HIS:NE2	1:E:696:VAL:HG22	2.35	0.41
1:A:423:VAL:HG12	1:A:425:LEU:H	1.85	0.41
1:A:642:ASP:OD1	1:A:859:SER:HA	2.20	0.41
1:B:428:GLY:HA3	2:B:1101:MKG:F1	2.11	0.41
1:C:780:TYR:OH	1:C:939:PRO:O	2.31	0.41
1:E:811:THR:O	1:E:819:ILE:HG13	2.21	0.41
1:B:351:LEU:HA	1:B:351:LEU:HD13	1.98	0.41
1:B:738:TYR:HB3	1:B:940:VAL:CG1	2.50	0.41
1:B:936:ILE:HG12	1:B:936:ILE:H	1.74	0.41
1:D:783:ILE:HG23	1:D:784:PRO:HD2	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:969:ASN:C	1:E:971:GLU:H	2.24	0.41
1:A:740:TYR:HA	1:A:780:TYR:HB2	2.03	0.41
1:A:391:ARG:HA	1:A:392:PRO:C	2.41	0.41
1:B:450:HIS:CG	1:B:451:PRO:HA	2.56	0.41
1:C:477:VAL:O	1:C:645:SER:N	2.52	0.41
1:A:633:TYR:OH	1:B:962:LYS:HB2	2.21	0.41
1:A:749:CYS:O	1:A:810:ARG:NH1	2.50	0.41
1:B:759:ILE:O	1:B:763:ILE:HG13	2.21	0.41
1:C:671:SER:HA	1:C:674:ARG:O	2.21	0.41
1:C:745:PHE:O	1:C:876:ILE:HB	2.21	0.41
1:B:921:CYS:O	1:B:925:VAL:HG22	2.21	0.40
1:C:810:ARG:NH2	1:C:810:ARG:HG2	2.36	0.40
1:E:338:HIS:HB2	1:E:342:SER:O	2.21	0.40
1:E:967:LEU:HD13	1:E:978:LEU:HD11	2.03	0.40
1:E:959:ILE:HD12	1:E:998:GLU:HG3	2.02	0.40
1:F:414:ARG:NH2	1:F:679:PRO:HG3	2.36	0.40
1:B:382:TRP:CE3	1:B:483:ALA:HB1	2.56	0.40
1:B:474:VAL:HG22	1:B:648:HIS:HD2	1.86	0.40
1:D:408:LYS:HD2	1:D:408:LYS:HA	1.79	0.40
1:F:356:VAL:HG12	1:F:357:ASN:ND2	2.37	0.40
1:A:735:SER:O	1:A:766:ARG:NH1	2.54	0.40
1:F:725:HIS:CE1	1:F:757:ASN:HA	2.57	0.40
1:B:408:LYS:HA	1:B:408:LYS:HD2	1.76	0.40
1:E:418:MET:HE1	1:E:662:ARG:HB3	2.04	0.40

All (3) 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:C:1027:GLU:OE2	2:B:1101:MKG:N1[1_655]	1.30	0.90
1:C:1027:GLU:OE2	2:B:1101:MKG:C4[1_655]	2.17	0.03
1:C:1027:GLU:OE2	2:B:1101:MKG:C15[1_655]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/647 (88%)	540 (95%)	26 (5%)	0	100	100
1	B	559/647 (86%)	537 (96%)	22 (4%)	0	100	100
1	C	562/647 (87%)	542 (96%)	18 (3%)	2 (0%)	34	69
1	D	550/647 (85%)	530 (96%)	20 (4%)	0	100	100
1	E	544/647 (84%)	523 (96%)	21 (4%)	0	100	100
1	F	486/647 (75%)	468 (96%)	18 (4%)	0	100	100
All	All	3267/3882 (84%)	3140 (96%)	125 (4%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	798	GLY
1	C	394	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	454/553 (82%)	446 (98%)	8 (2%)	59	82
1	B	467/553 (84%)	463 (99%)	4 (1%)	78	91
1	C	445/553 (80%)	435 (98%)	10 (2%)	52	79
1	D	446/553 (81%)	437 (98%)	9 (2%)	55	80
1	E	337/553 (61%)	335 (99%)	2 (1%)	86	94
1	F	252/553 (46%)	243 (96%)	9 (4%)	35	69
All	All	2401/3318 (72%)	2359 (98%)	42 (2%)	60	83

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	467	LEU
1	A	481	ASP
1	A	629	PHE
1	A	674	ARG
1	A	860	LYS
1	A	895	ASP
1	A	913	PHE
1	A	931	ASP
1	B	766	ARG
1	B	772	ARG
1	B	946	LYS
1	B	997	GLU
1	C	398	ARG
1	C	421	LYS
1	C	425	LEU
1	C	481	ASP
1	C	499	SER
1	C	632	ARG
1	C	719	TYR
1	C	728	TYR
1	C	766	ARG
1	C	930	ASP
1	D	446	LYS
1	D	728	TYR
1	D	746	PHE
1	D	801	LEU
1	D	805	MET
1	D	860	LYS
1	D	895	ASP
1	D	930	ASP
1	D	994	ARG
1	E	398	ARG
1	E	806	HIS
1	F	466	LYS
1	F	481	ASP
1	F	488	ASP
1	F	612	CYS
1	F	662	ARG
1	F	745	PHE
1	F	829	ASN
1	F	878	ASP
1	F	887	SER

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



sidechains are listed below:

Mol	Chain	Res	Type
1	C	357	ASN
1	C	858	HIS
1	C	983	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	MKG	A	1101	-	33,35,35	0.36	0	34,50,50	0.37	0
2	MKG	B	1101	-	33,35,35	0.34	0	34,50,50	0.45	0
2	MKG	C	1101	-	33,35,35	0.35	0	34,50,50	0.35	0
2	MKG	D	1101	-	33,35,35	0.35	0	34,50,50	0.32	0
2	MKG	E	1101	-	33,35,35	0.33	0	34,50,50	0.38	0
2	MKG	F	1101	-	33,35,35	0.33	0	34,50,50	0.30	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	MKG	A	1101	-	-	1/16/44/44	0/4/4/4
2	MKG	B	1101	-	-	1/16/44/44	0/4/4/4
2	MKG	C	1101	-	-	1/16/44/44	0/4/4/4
2	MKG	D	1101	-	-	1/16/44/44	0/4/4/4
2	MKG	E	1101	-	-	1/16/44/44	0/4/4/4
2	MKG	F	1101	-	-	2/16/44/44	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1101	MKG	C6-C5-N1-C4
2	F	1101	MKG	C5-C6-N2-C8
2	A	1101	MKG	C5-C6-N2-C8
2	B	1101	MKG	C5-C6-N2-C8
2	C	1101	MKG	C5-C6-N2-C8
2	D	1101	MKG	C5-C6-N2-C8
2	E	1101	MKG	C5-C6-N2-C8

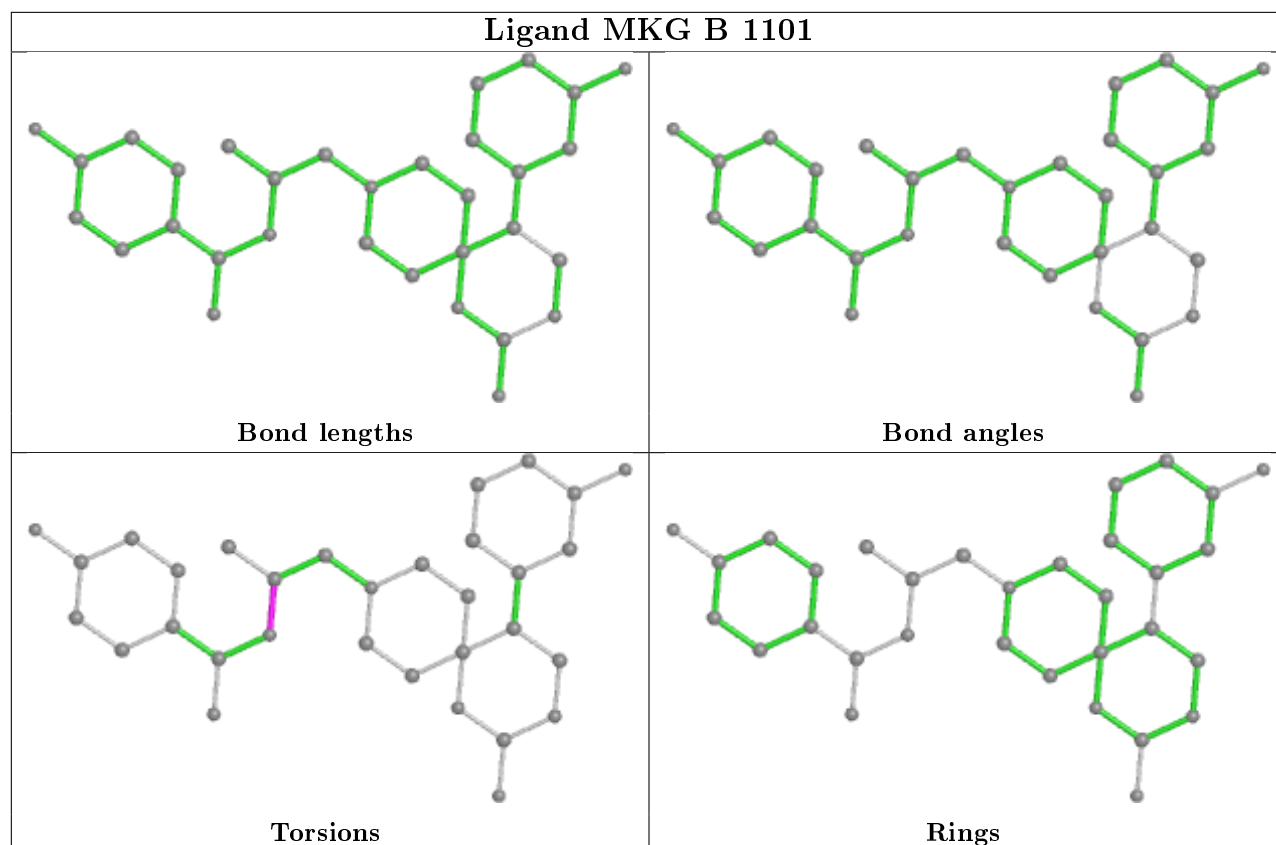
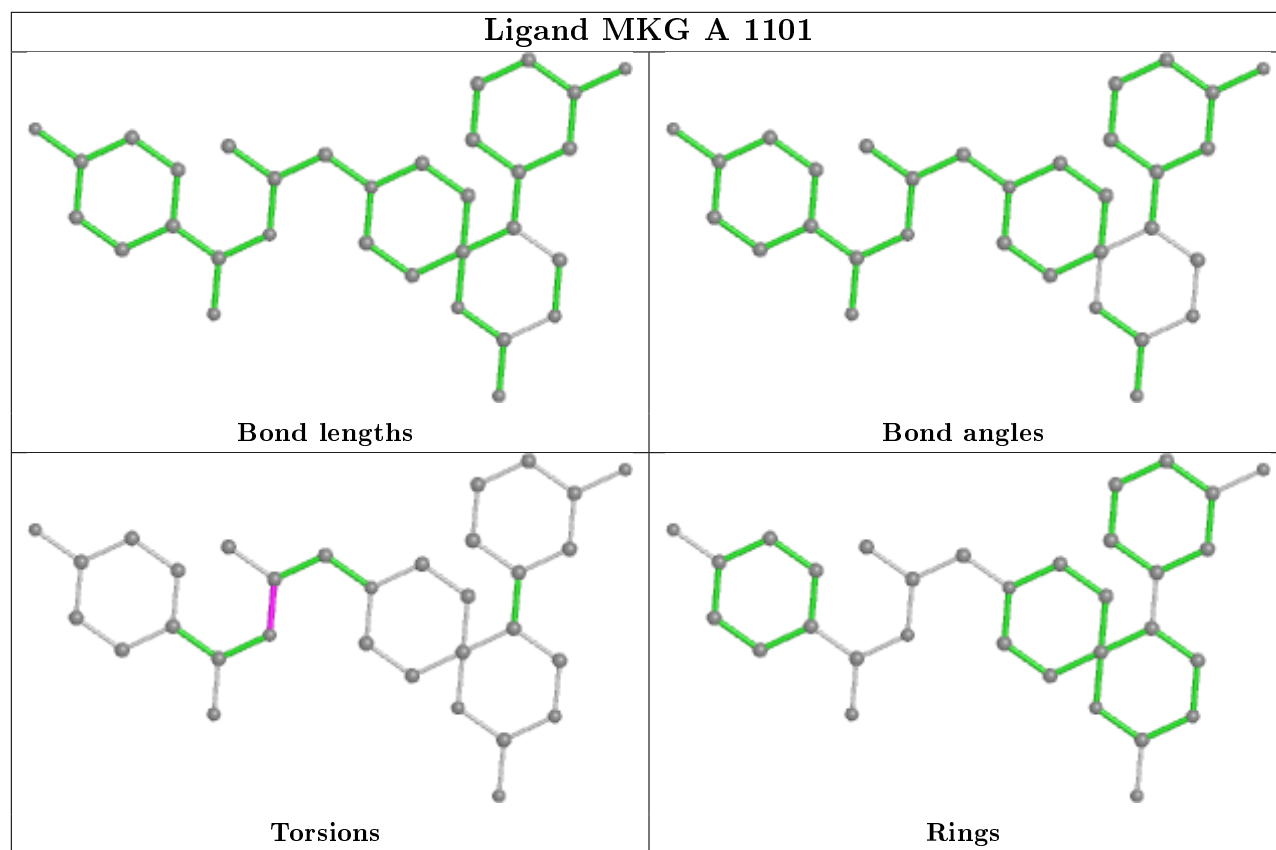
There are no ring outliers.

3 monomers are involved in 6 short contacts:

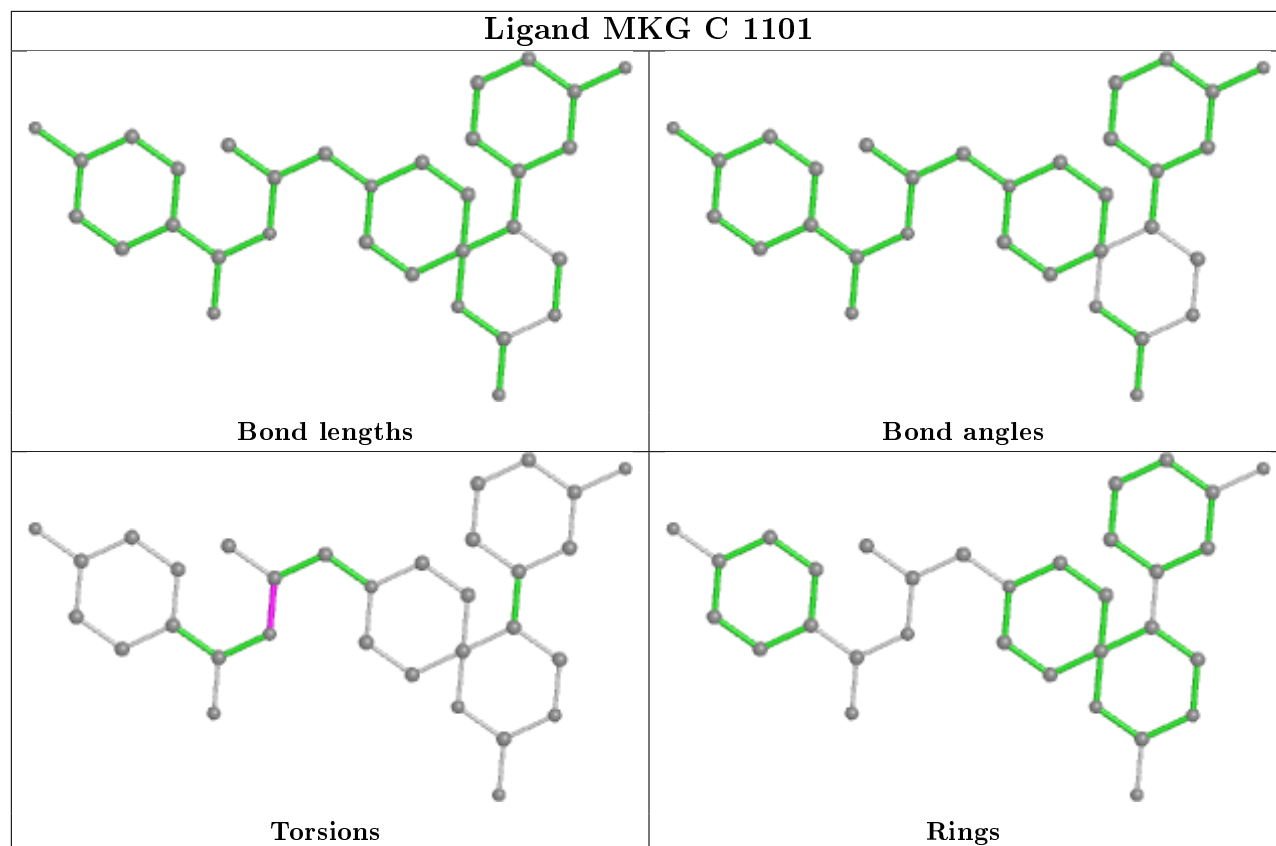
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	MKG	1	0
2	B	1101	MKG	1	3
2	D	1101	MKG	1	0

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

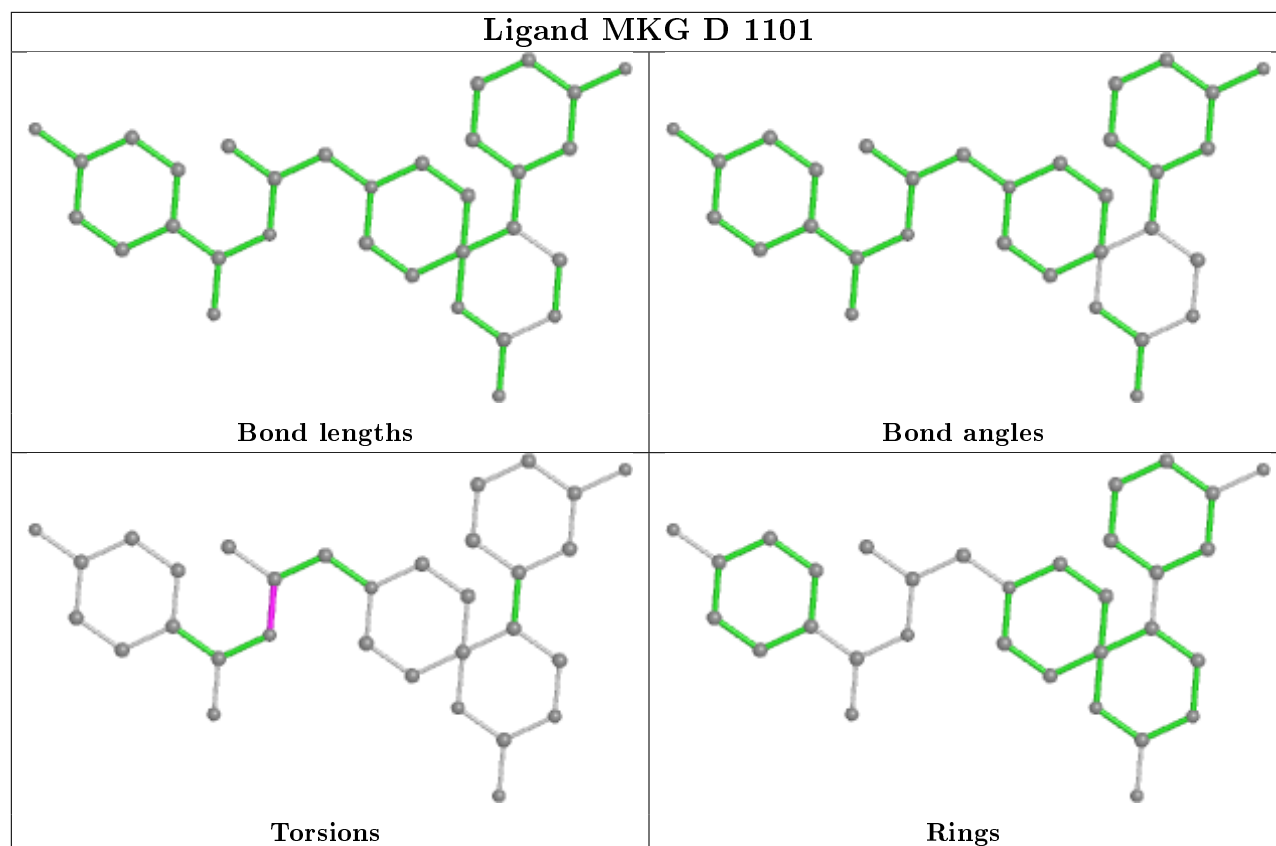
equivalents in the CSD to analyse the geometry.



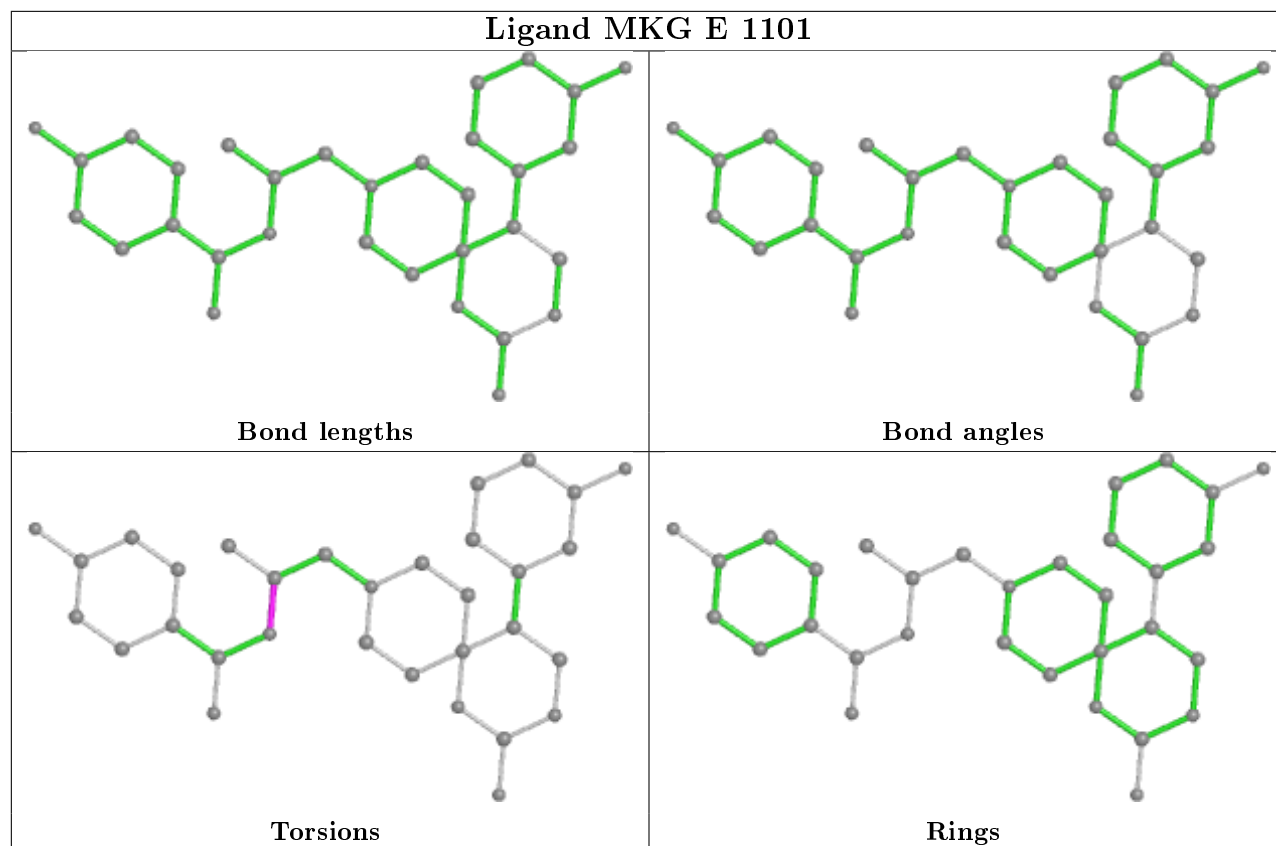
## Ligand MKG C 1101



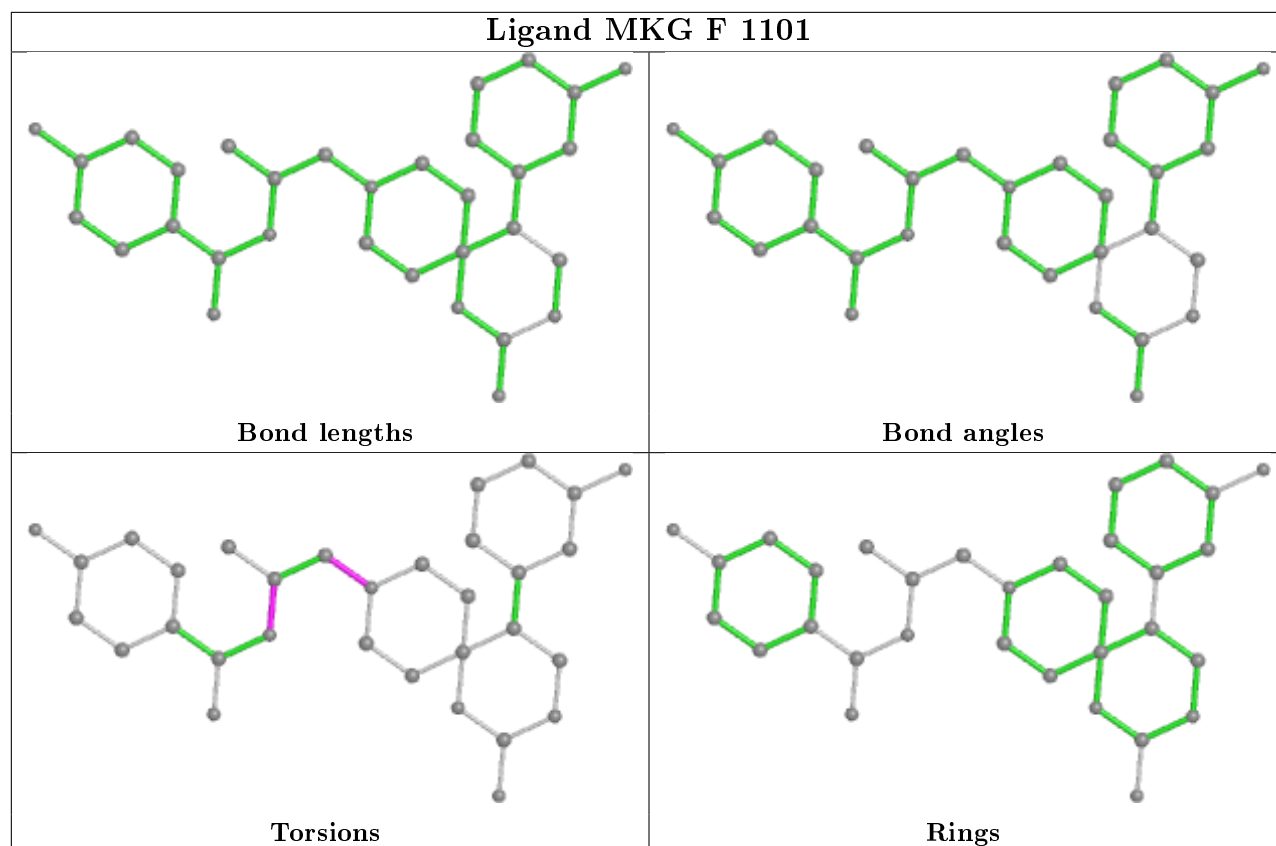
## Ligand MKG D 1101



## Ligand MKG E 1101



## Ligand MKG F 1101



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	576/647 (89%)	-0.20	2 (0%) 94 92	27, 46, 76, 119	0
1	B	569/647 (87%)	-0.19	5 (0%) 84 75	26, 43, 72, 116	0
1	C	572/647 (88%)	-0.22	3 (0%) 91 86	25, 40, 67, 122	0
1	D	564/647 (87%)	-0.18	5 (0%) 84 75	28, 48, 77, 118	0
1	E	560/647 (86%)	0.23	23 (4%) 37 24	46, 83, 116, 179	0
1	F	526/647 (81%)	0.53	55 (10%) 6 3	60, 96, 139, 160	0
All	All	3367/3882 (86%)	-0.01	93 (2%) 53 37	25, 53, 113, 179	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	850	LEU	4.1
1	F	845	GLU	4.1
1	F	344	ALA	4.0
1	F	883	GLY	4.0
1	F	904	ASP	4.0
1	F	949	TRP	4.0
1	F	868	THR	3.9
1	F	1021	PRO	3.9
1	B	682	LEU	3.7
1	F	853	GLU	3.7
1	F	978	LEU	3.5
1	F	851	VAL	3.4
1	E	848	GLY	3.3
1	E	849	ASN	3.3
1	E	983	ASN	3.3
1	E	990	GLU	3.3
1	B	985	PRO	3.2
1	E	844	ALA	3.2
1	F	968	PRO	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	681	LEU	3.2
1	E	679	PRO	3.2
1	E	663	TRP	3.1
1	F	841	ARG	3.1
1	F	852	THR	3.1
1	E	497	VAL	3.1
1	E	681	LEU	3.0
1	E	607	HIS	3.0
1	F	495	THR	3.0
1	F	498	GLY	2.9
1	E	496	ASP	2.9
1	F	846	LEU	2.9
1	F	494	LEU	2.9
1	F	405	LEU	2.8
1	F	750	ALA	2.8
1	C	983	ASN	2.8
1	F	832	ILE	2.8
1	F	443	PRO	2.8
1	F	442	HIS	2.7
1	E	495	THR	2.7
1	F	941	SER	2.6
1	F	412	GLY	2.6
1	F	1017	GLU	2.6
1	F	964	PHE	2.6
1	D	985	PRO	2.6
1	F	848	GLY	2.5
1	B	848	GLY	2.5
1	F	831	TRP	2.5
1	F	758	LYS	2.5
1	E	418	MET	2.4
1	F	416	PHE	2.4
1	F	341	GLY	2.4
1	E	982	ILE	2.4
1	F	679	PRO	2.4
1	F	844	ALA	2.4
1	F	842	THR	2.4
1	F	830	GLN	2.4
1	B	849	ASN	2.4
1	F	706	LEU	2.4
1	E	988	ALA	2.4
1	F	967	LEU	2.4
1	D	991	ASP	2.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	985	PRO	2.3
1	F	350	ALA	2.3
1	F	762	ALA	2.3
1	F	811	THR	2.2
1	C	752	ASP	2.2
1	F	413	VAL	2.2
1	F	635	THR	2.2
1	D	850	LEU	2.2
1	E	963	VAL	2.2
1	E	680	PHE	2.2
1	F	445	ILE	2.2
1	A	980	ASP	2.2
1	E	992	PRO	2.2
1	F	444	ASN	2.2
1	F	707	LEU	2.2
1	A	994	ARG	2.2
1	E	682	LEU	2.1
1	C	673	TYR	2.1
1	F	342	SER	2.1
1	E	702	ALA	2.1
1	D	453	HIS	2.1
1	F	373	ASN	2.1
1	F	945	PHE	2.1
1	D	965	ARG	2.1
1	F	710	ALA	2.1
1	F	954	ALA	2.1
1	F	675	SER	2.1
1	E	374	GLU	2.0
1	F	836	SER	2.0
1	E	995	ALA	2.0
1	F	633	TYR	2.0
1	F	999	LEU	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 ⓘ

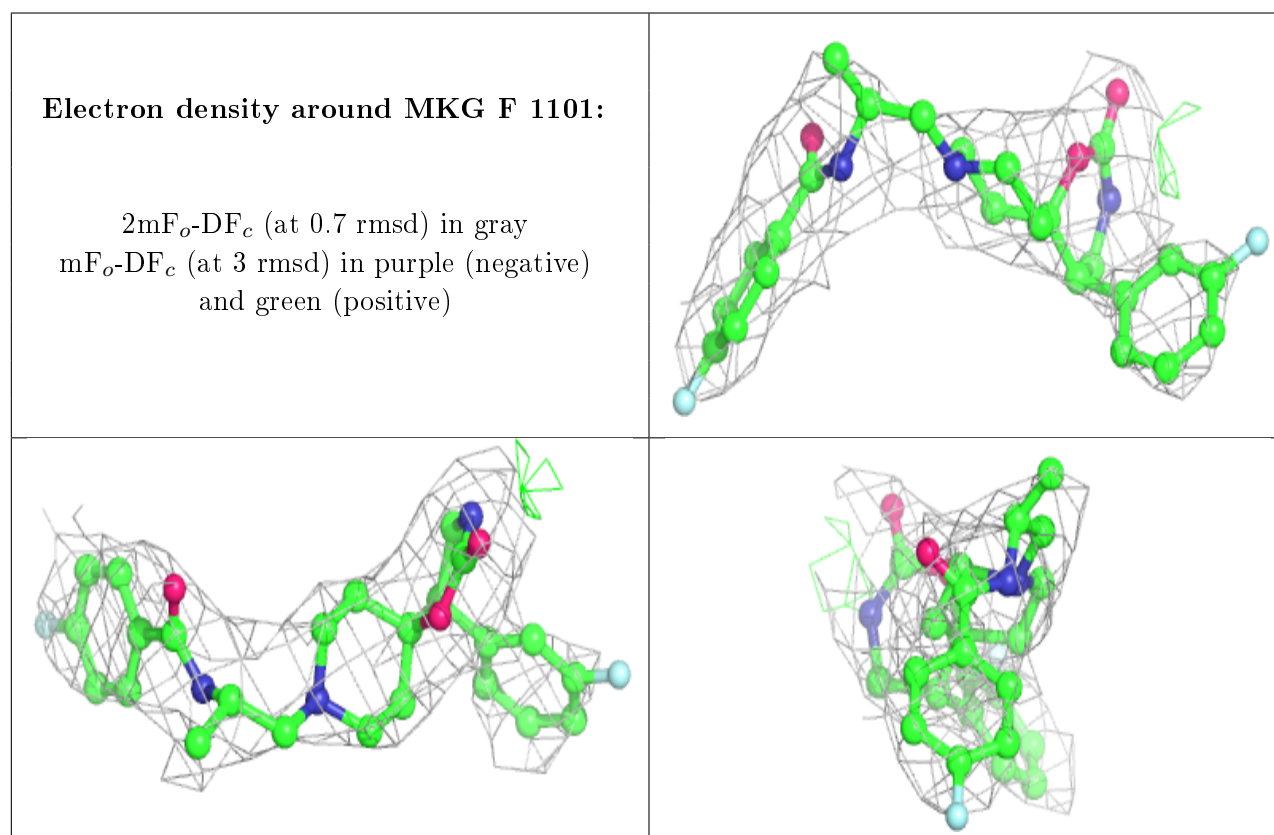
There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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.

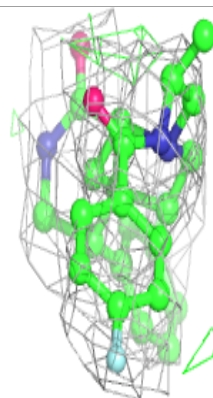
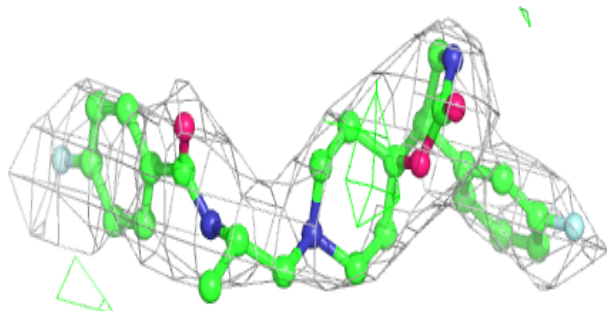
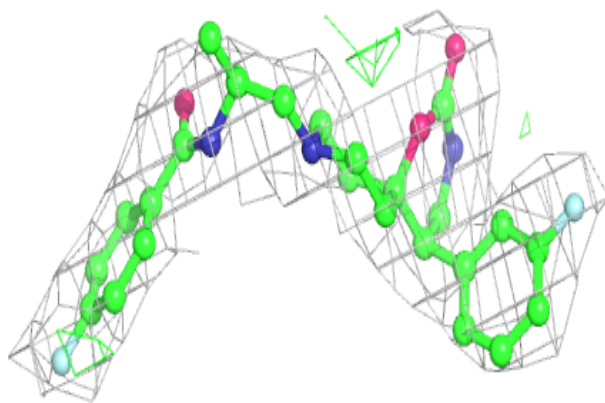
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MKG	F	1101	32/32	0.89	0.27	66,78,89,90	0
2	MKG	E	1101	32/32	0.90	0.24	67,74,89,92	0
2	MKG	B	1101	32/32	0.93	0.21	29,39,48,56	0
2	MKG	C	1101	32/32	0.93	0.22	31,38,46,60	0
2	MKG	A	1101	32/32	0.94	0.23	34,43,57,71	0
2	MKG	D	1101	32/32	0.94	0.23	33,42,49,74	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.

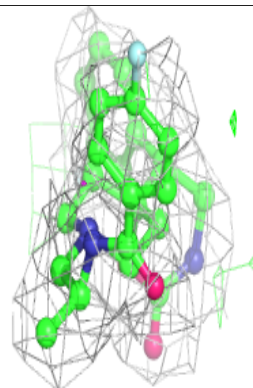
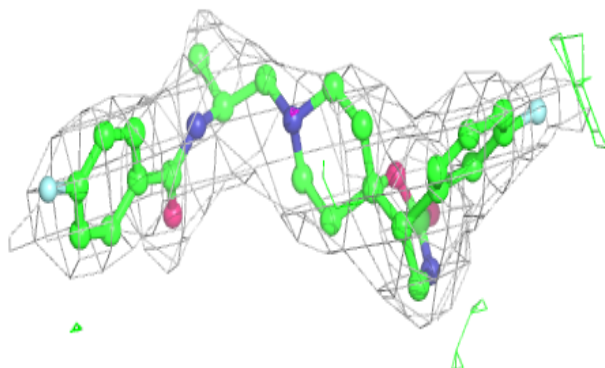
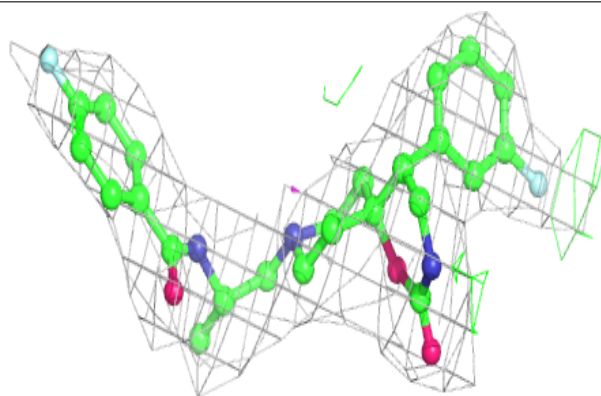


**Electron density around MKG E 1101:**

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

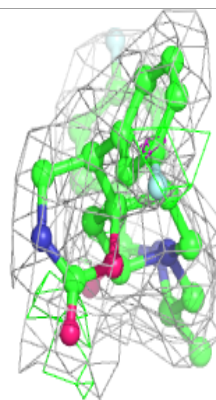
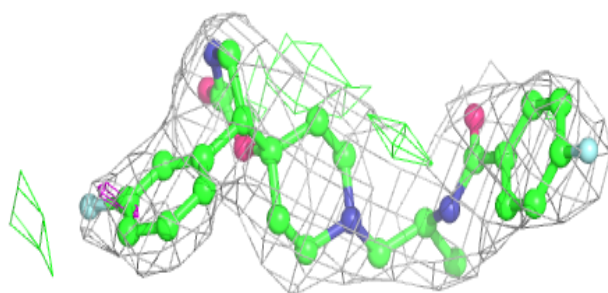
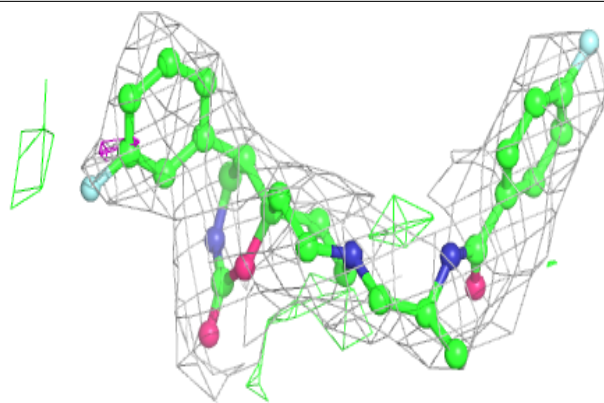
**Electron density around MKG B 1101:**

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

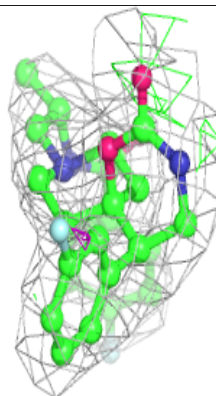
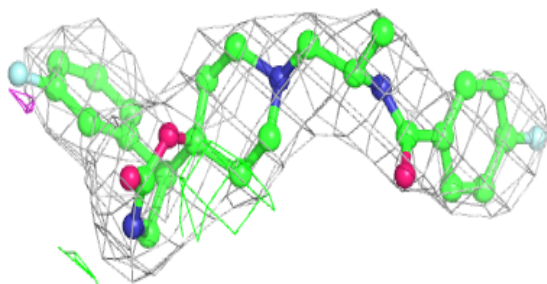
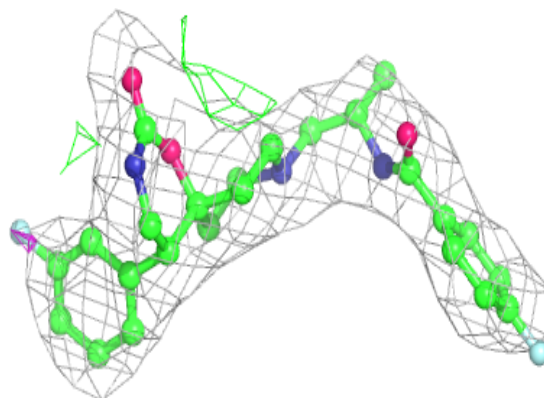


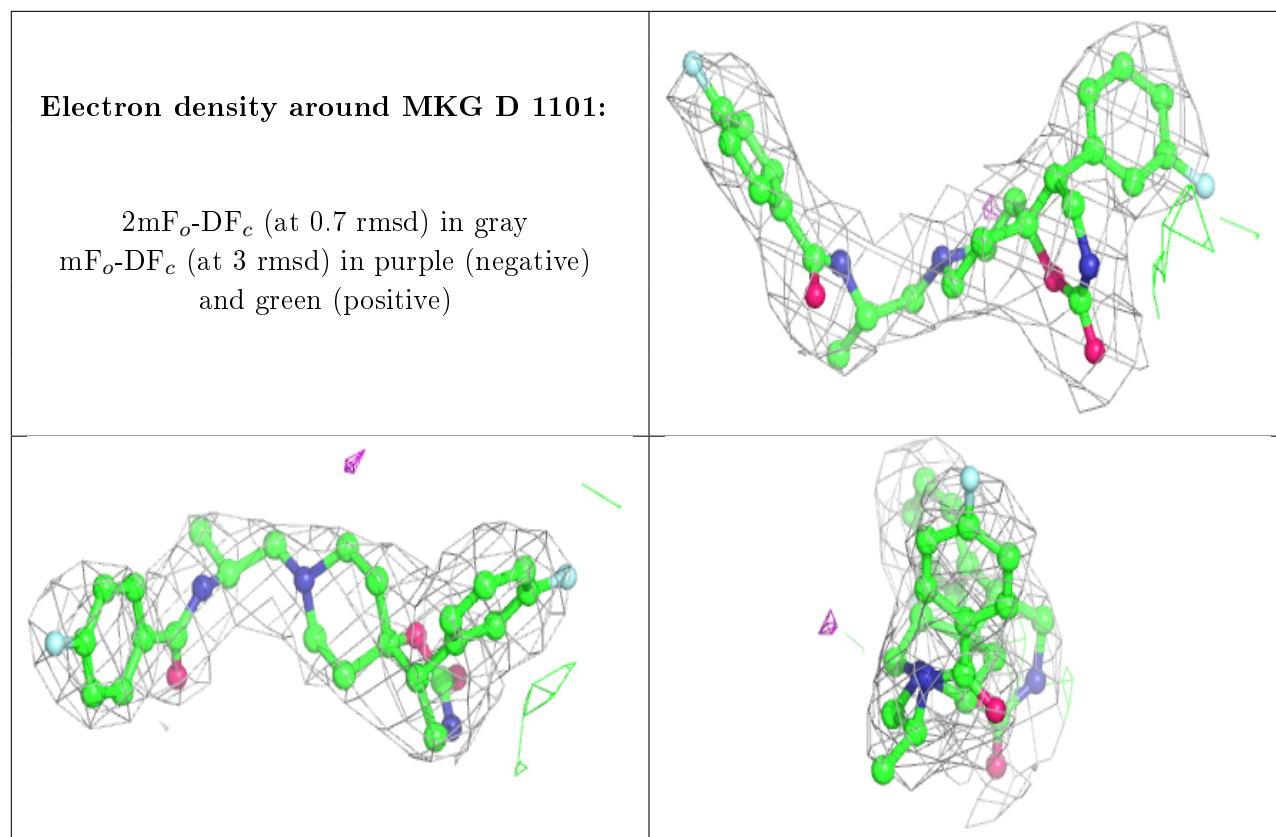
**Electron density around MKG C 1101:**

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

**Electron density around MKG A 1101:**

$2mF_o-DF_c$  (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.