



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:11 PM UTC

PDB ID : 6OHR / pdb_00006ohr
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

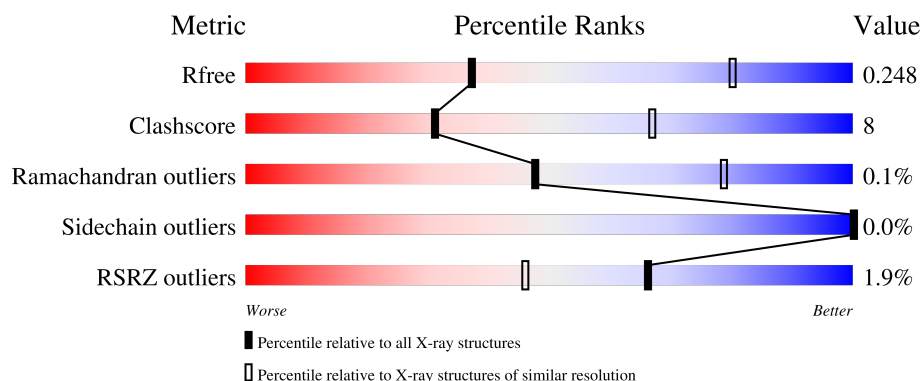
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 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 $\leq 5\%$. 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	71% 18% 11%
1	B	647	67% 21% 12%
1	C	647	73% 16% 12%
1	D	647	70% 17% 13%
1	E	647	3% 71% 16% 13%

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Mol	Chain	Length	Quality of chain
1	F	647	5% 68% 13% 19%

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

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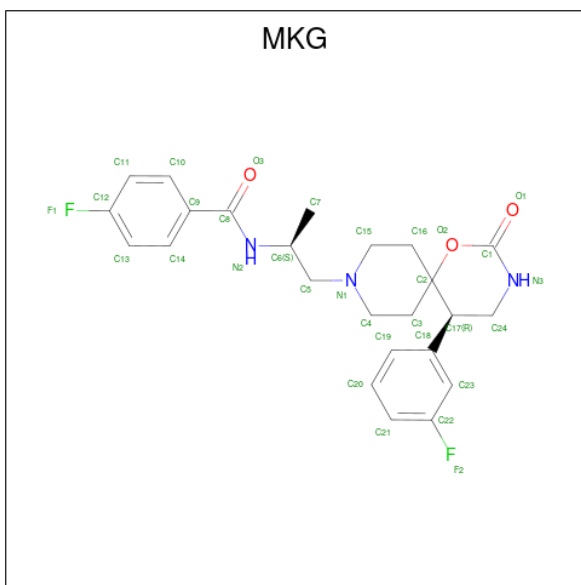
Chain	Residue	Modelled	Actual	Comment	Reference
B	580	GLY	VAL	linker	UNP Q13393
B	581	SER	LYS	linker	UNP Q13393
B	582	GLY	ARG	linker	UNP Q13393
B	583	SER	VAL	linker	UNP Q13393
B	584	GLY	THR	linker	UNP Q13393
B	587	SER	PRO	linker	UNP Q13393
B	588	GLY	SER	linker	UNP Q13393
B	589	SER	LEU	linker	UNP Q13393
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

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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

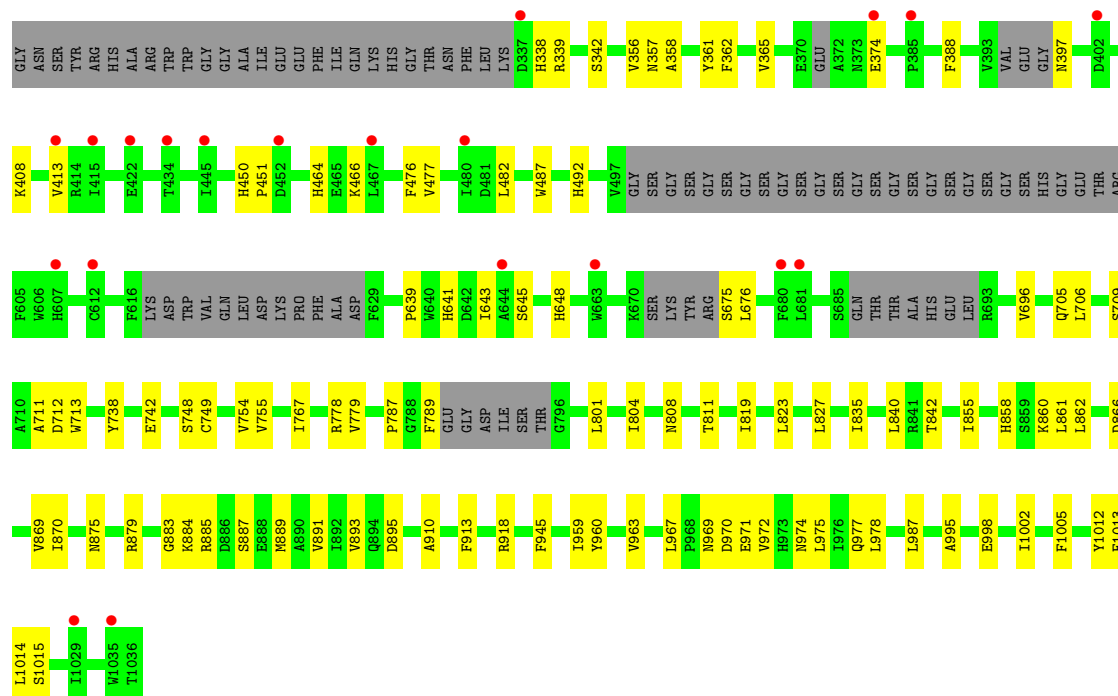
- Molecule 2 is 4-fluoro-N-{(2S)-1-[(5R)-5-(3-fluorophenyl)-2-oxo-1-oxa-3,9-diazaspiro[5.5]undecan-9-yl]propan-2-yl}benzamide (CCD ID: MKG) (formula: C₂₄H₂₇F₂N₃O₃) (labeled as "Ligand of Interest" by depositor).



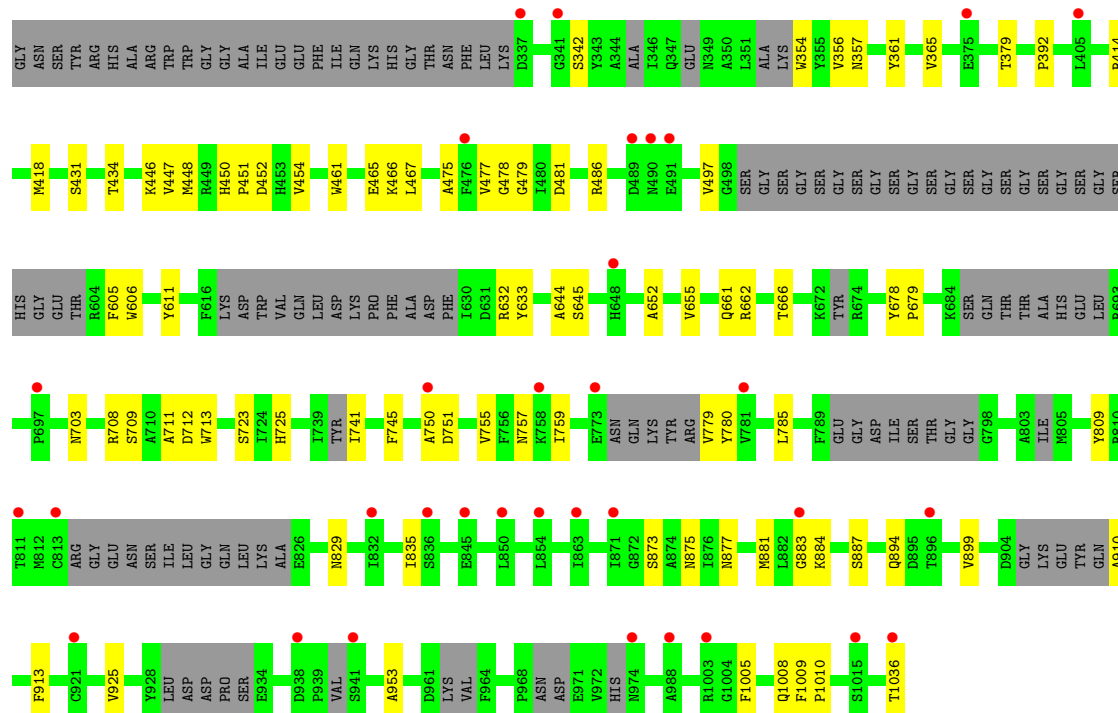
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 32	C 24	F 2	N 3	O 3	0	0
2	B	1	Total 32	C 24	F 2	N 3	O 3	0	0
2	C	1	Total 32	C 24	F 2	N 3	O 3	0	0
2	D	1	Total 32	C 24	F 2	N 3	O 3	0	0
2	E	1	Total 32	C 24	F 2	N 3	O 3	0	0
2	F	1	Total 32	C 24	F 2	N 3	O 3	0	0

- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.14_3211: ???)	Depositor
R, R_{free}	0.221 , 0.247 0.222 , 0.248	Depositor DCC
R_{free} test set	6615 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	25872	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.14	0/4649	0.35	0/6325
1	B	0.13	0/4671	0.35	0/6341
1	C	0.14	0/4617	0.34	0/6279
1	D	0.14	0/4573	0.35	0/6214
1	E	0.14	0/4148	0.35	0/5677
1	F	0.13	0/3653	0.34	0/4994
All	All	0.13	0/26311	0.35	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	77	0
1	B	4557	0	4361	88	0
1	C	4503	0	4254	59	3
1	D	4461	0	4218	69	0
1	E	4045	0	3405	66	0
1	F	3580	0	2781	49	0
2	A	32	0	0	1	0

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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	404	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 (404) 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:439:MET:HE3	1:C:446:LYS:HA	1.74	0.70
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:439:MET:HE3	1:D:446:LYS:HA	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:ARG:HB3	1:E:705:GLN:HE22	1.61	0.65
1:E:641:HIS:NE2	1:E:742:GLU:OE2	2.27	0.65
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:B:653:ARG:HH11	1:B:684:LYS:C	2.09	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:D:738:TYR:OH	1:D:866:ASP:OD1	2.19	0.60
1:A:464:HIS:O	1:A:466:LYS:NZ	2.31	0.59
1:D:464:HIS:O	1:D:466:LYS:NZ	2.33	0.59
1:A:738:TYR:OH	1:A:866:ASP:OD1	2.20	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:B:464:HIS:O	1:B:466:LYS:NZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ILE:HD13	1:A:438:LEU:HD13	1.88	0.56
1:B:738:TYR:OH	1:B:866:ASP:OD1	2.20	0.55
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:F:466:LYS:HD2	1:F:479:GLY:C	2.31	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
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:D:448:MET:HE2	1:D:663:TRP:CD2	2.43	0.53
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:B:807:PHE:HZ	1:B:1032:MET:HE3	1.73	0.53
1:F:703:ASN:N	1:F:894:GLN:O	2.38	0.53
1:A:970:ASP:OD1	1:A:970:ASP:N	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:783:ILE:HD11	1:B:812:MET:HE1	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:VAL:CG2	1:A:395:GLU:H	2.13	0.52
1:A:735:SER:HG	1:A:777:TYR:HH	1.44	0.52
1:B:660:ILE:HG12	1:B:681:LEU:HB3	1.91	0.52
1:C:709:SER:O	1:C:887:SER:HA	2.09	0.52
1:C:860:LYS:HD3	1:C:873:SER:HA	1.91	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:D:615:VAL:HG12	1:D:638:MET:HE3	1.89	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
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:356:VAL:HA	1:E:643:ILE:HD13	1.93	0.51
1:E:970:ASP:HB3	1:E:1012:TYR:H	1.75	0.51
1:A:737:HIS:CD2	1:A:903:MET:HE3	2.46	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:784:PRO:HD3	1:D:857:VAL:HB	1.92	0.51
1:D:875:ASN:ND2	2:D:1101:MKG:O1	2.42	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:C:738:TYR:OH	1:C:866:ASP:OD1	2.29	0.51
1:D:866:ASP:HB3	1:D:910:ALA:HB1	1.93	0.50
1:A:643:ILE:HG21	1:A:861:LEU:HD13	1.92	0.50
1:A:776:LYS:HD3	1:A:778:ARG:HH21	1.74	0.50
1:A:931:ASP:CG	1:A:932:PRO:HD2	2.37	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:362:PHE:HE1	1:E:482:LEU:HD23	1.77	0.49
1:E:388:PHE:HE1	1:E:397:ASN:HA	1.78	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:E:706:LEU:HD22	1:E:889:MET:HE1	1.95	0.48
1:C:495:THR:HG22	1:C:846:LEU:HB2	1.94	0.48
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:B:812:MET:HE3	1:B:812:MET:HB2	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ASP:O	1:C:632:ARG:HD2	2.15	0.47
1:C:606:TRP:O	1:C:632:ARG:NH1	2.32	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:D:960:TYR:CZ	1:D:1002:ILE:HD13	2.49	0.47
1:E:970:ASP:HB2	1:E:1012:TYR:HB2	1.95	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: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
1:A:391:ARG:HA	1:A:392:PRO:C	2.41	0.46
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:O	1:E:858:HIS:ND1	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:F:418:MET:HE3	1:F:662:ARG:NH1	2.31	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:A:737:HIS:CG	1:A:903:MET:HE3	2.51	0.46
1:B:402:ASP:OD1	1:B:403:CYS:N	2.49	0.46
1:B:974:ASN:HB2	1:B:977:GLN:HG3	1.97	0.46
1:C:464:HIS:O	1:C:466:LYS:NZ	2.44	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:E:969:ASN:C	1:E:971:GLU:H	2.24	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:709:SER:O	1:E:887:SER:HA	2.16	0.45
1:E:823:LEU:HB3	1:E:827:LEU:HD11	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:739:ILE:HG13	1:D:862:LEU:HD11	1.98	0.45
1:D:968:PRO:HB2	1:D:1010:PRO:HG3	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:B:805:MET:HE3	1:B:809:TYR:HE2	1.81	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:636:PRO:HG3	1:D:851:VAL:HB	1.99	0.44
1:D:746:PHE:HB2	1:D:783:ILE:CD1	2.47	0.44
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: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:F:809:TYR:OH	1:F:1010:PRO:O	2.36	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:446:LYS:HD3	1:C:678:TYR:HD1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:ASP:HA	1:C:859:SER:HB3	2.00	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:B:648:HIS:HE2	1:B:696:VAL:H	1.66	0.43
1:F:448:MET:HE3	1:F:666:THR: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
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:339:ARG:NH1	1:B:894:GLN:OE1	2.51	0.43
1:B:383:LEU:HD22	1:B:438:LEU:HD11	2.00	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:A:812:MET:HE3	1:A:812:MET:HB2	1.86	0.43
1:B:418:MET:HE2	1:B:659:PHE:CE1	2.53	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:391:ARG:HE	1:D:487:TRP:CG	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:SER:HA	1:A:674:ARG:O	2.19	0.43
1:B:391:ARG:HA	1:B:392:PRO:C	2.44	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:E:639:PRO:HB2	1:E:855:ILE:HG23	2.02	0.42
1:E:842:THR:HB	1:E:1005:PHE:HD1	1.84	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
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:492:HIS:HD2	1:B:855:ILE:HD13	1.84	0.42
1:B:776:LYS:HD2	1:B:778:ARG:NH2	2.35	0.42
1:C:448:MET:HE2	1:C:678:TYR:HD2	1.85	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:OD1	1:F:712:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:862:LEU:HD23	1:B:870:ILE:HD12	2.02	0.41
1:C:665:PHE:HE1	1:C:669:MET:HE2	1.85	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:B:934:GLU:H	1:B:934:GLU:CD	2.26	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:A:913:PHE:CD1	1:A:913:PHE:C	2.99	0.41
1:B:351:LEU:HD13	1:B:351:LEU:HA	1.98	0.41
1:B:738:TYR:HB3	1:B:940:VAL:CG1	2.50	0.41
1:B:936:ILE:H	1:B:936:ILE:HG12	1.74	0.41
1:D:783:ILE:HG23	1:D:784:PRO:HD2	2.02	0.41
1:A:740:TYR:HA	1:A:780:TYR:HB2	2.03	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:959:ILE:HD12	1:E:998:GLU:HG3	2.02	0.40
1:E:967:LEU:HD13	1:E:978:LEU:HD11	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:VAL:HG22	1:B:648:HIS:HD2	1.86	0.40
1:D:408:LYS:HA	1:D:408:LYS:HD2	1.79	0.40
1:E:889:MET:HE3	1:E:889:MET:HB3	1.85	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

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%)	30	62
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%)	48	79

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%)	454 (100%)	0	100	100
1	B	467/553 (84%)	466 (100%)	1 (0%)	87	89
1	C	445/553 (80%)	445 (100%)	0	100	100
1	D	446/553 (81%)	446 (100%)	0	100	100
1	E	337/553 (61%)	337 (100%)	0	100	100
1	F	252/553 (46%)	252 (100%)	0	100	100
All	All	2401/3318 (72%)	2400 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	603	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	607	HIS
1	A	909	GLN
1	B	397	ASN
1	B	430	ASN
1	B	607	HIS
1	B	909	GLN
1	C	357	ASN
1	C	737	HIS
1	C	806	HIS
1	C	858	HIS
1	C	983	ASN

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Mol	Chain	Res	Type
1	D	453	HIS
1	D	833	ASN
1	E	338	HIS
1	E	357	ASN
1	E	492	HIS
1	E	730	HIS
1	E	734	ASN
1	E	771	HIS
1	E	843	HIS
1	E	909	GLN
1	E	920	GLN
1	F	357	ASN
1	F	397	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 oligosaccharides 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	F	1101	-	34,35,35	0.36	0	37,50,50	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MKG	C	1101	-	34,35,35	0.37	0	37,50,50	0.35	0
2	MKG	D	1101	-	34,35,35	0.37	0	37,50,50	0.34	0
2	MKG	A	1101	-	34,35,35	0.38	0	37,50,50	0.32	0
2	MKG	B	1101	-	34,35,35	0.37	0	37,50,50	0.39	0
2	MKG	E	1101	-	34,35,35	0.36	0	37,50,50	0.32	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	F	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	-	-	0/16/44/44	0/4/4/4
2	MKG	A	1101	-	-	0/16/44/44	0/4/4/4
2	MKG	B	1101	-	-	0/16/44/44	0/4/4/4
2	MKG	E	1101	-	-	0/16/44/44	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1101	MKG	C6-C5-N1-C4
2	C	1101	MKG	C6-C5-N1-C4

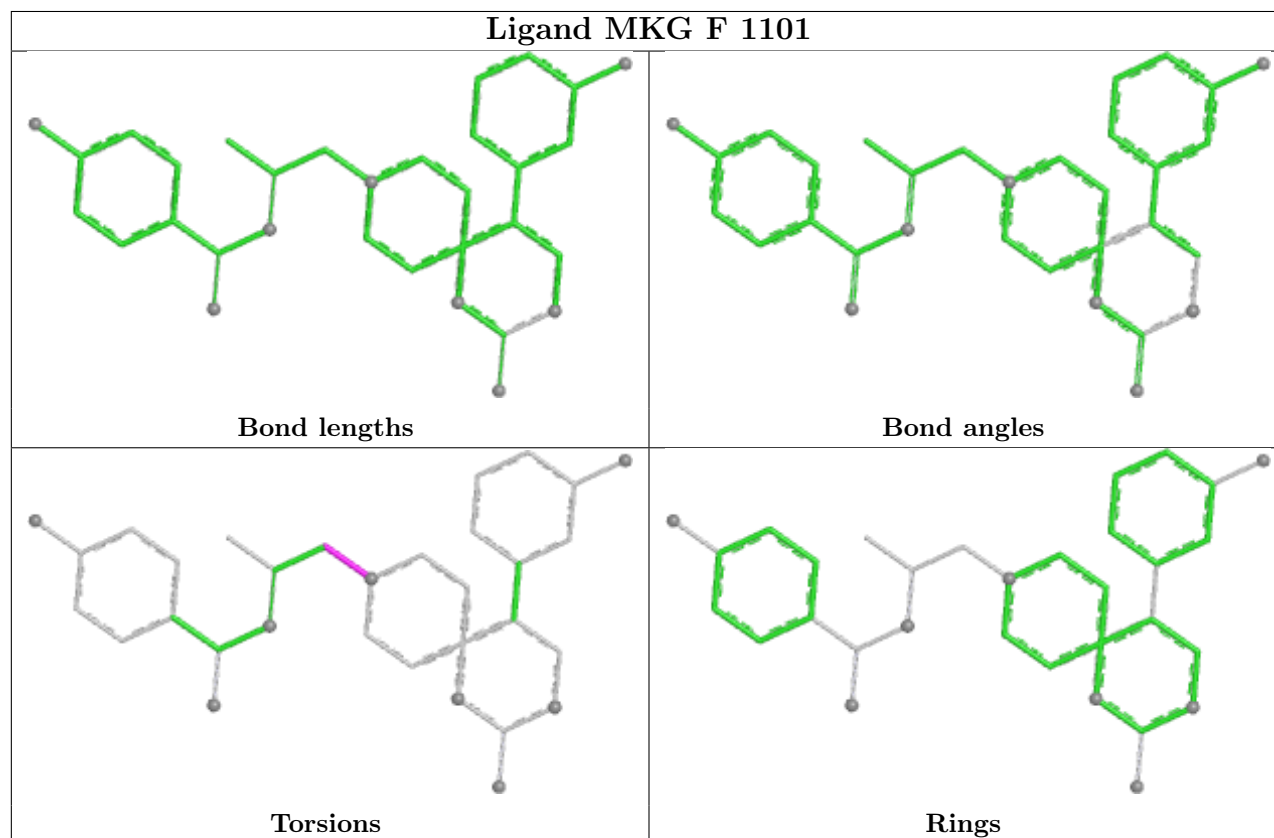
There are no ring outliers.

3 monomers are involved in 6 short contacts:

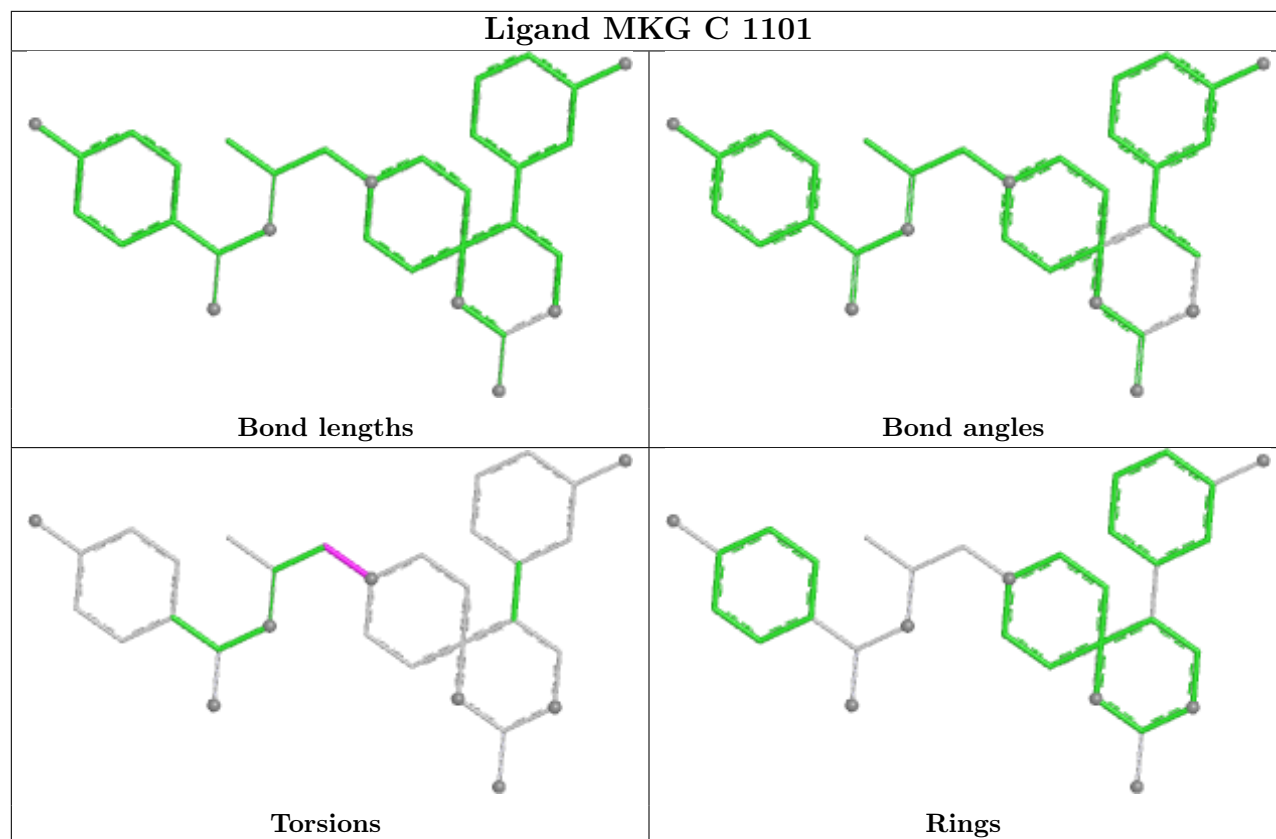
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1101	MKG	1	0
2	A	1101	MKG	1	0
2	B	1101	MKG	1	3

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.

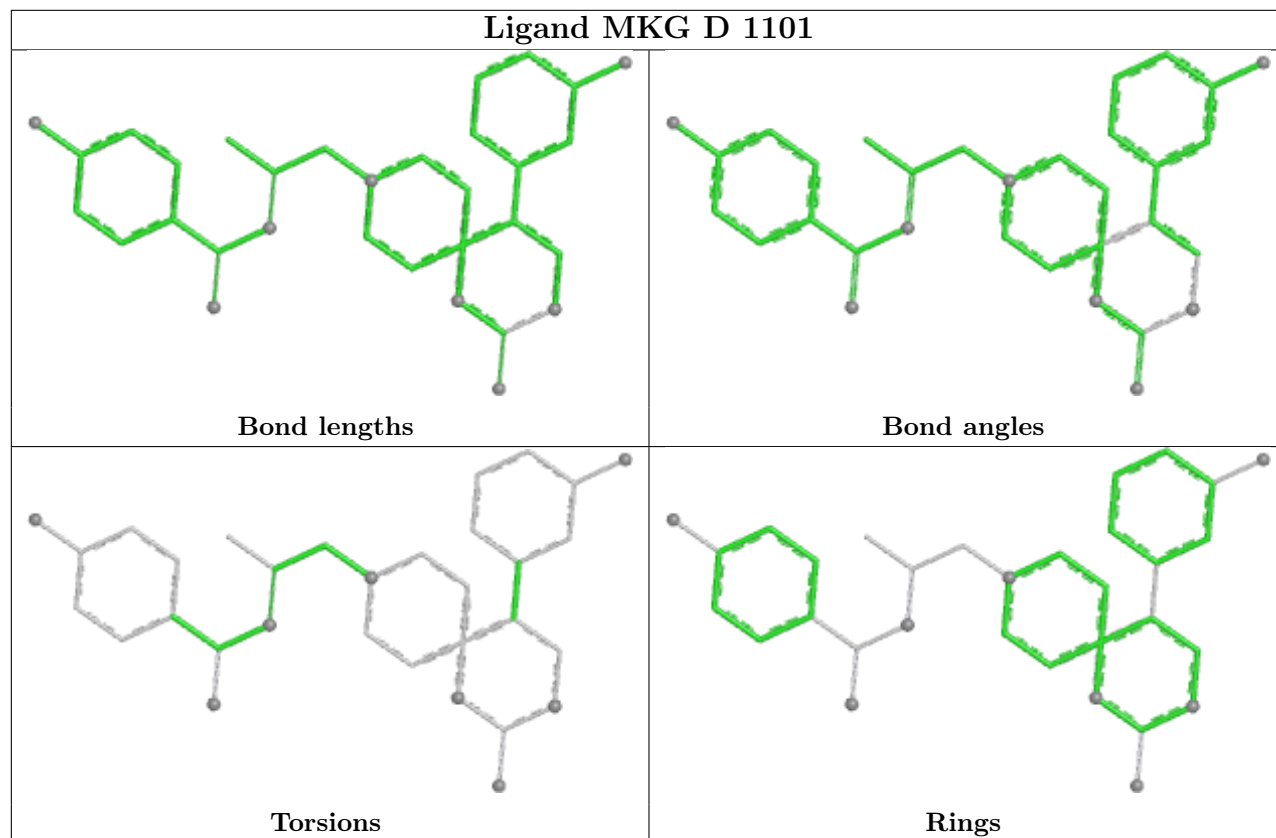
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



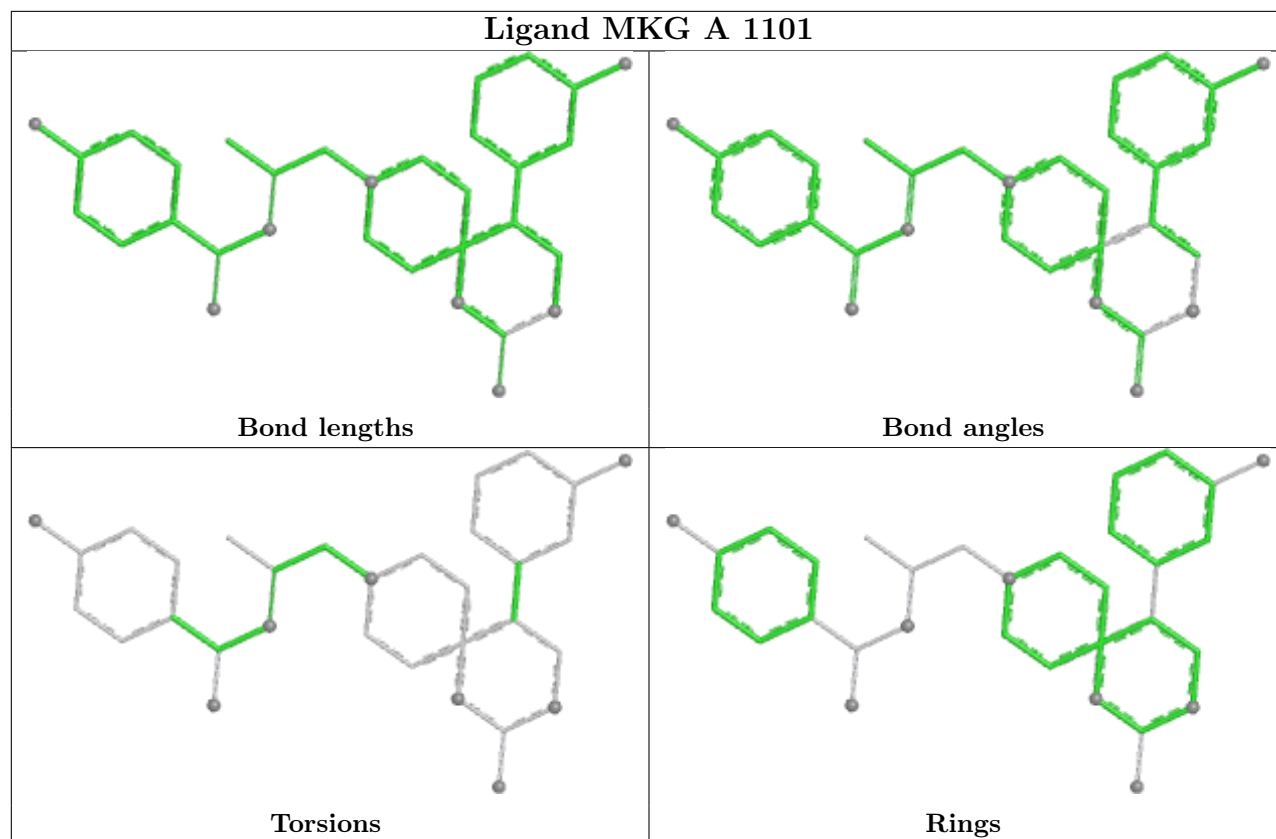
Ligand MKG C 1101



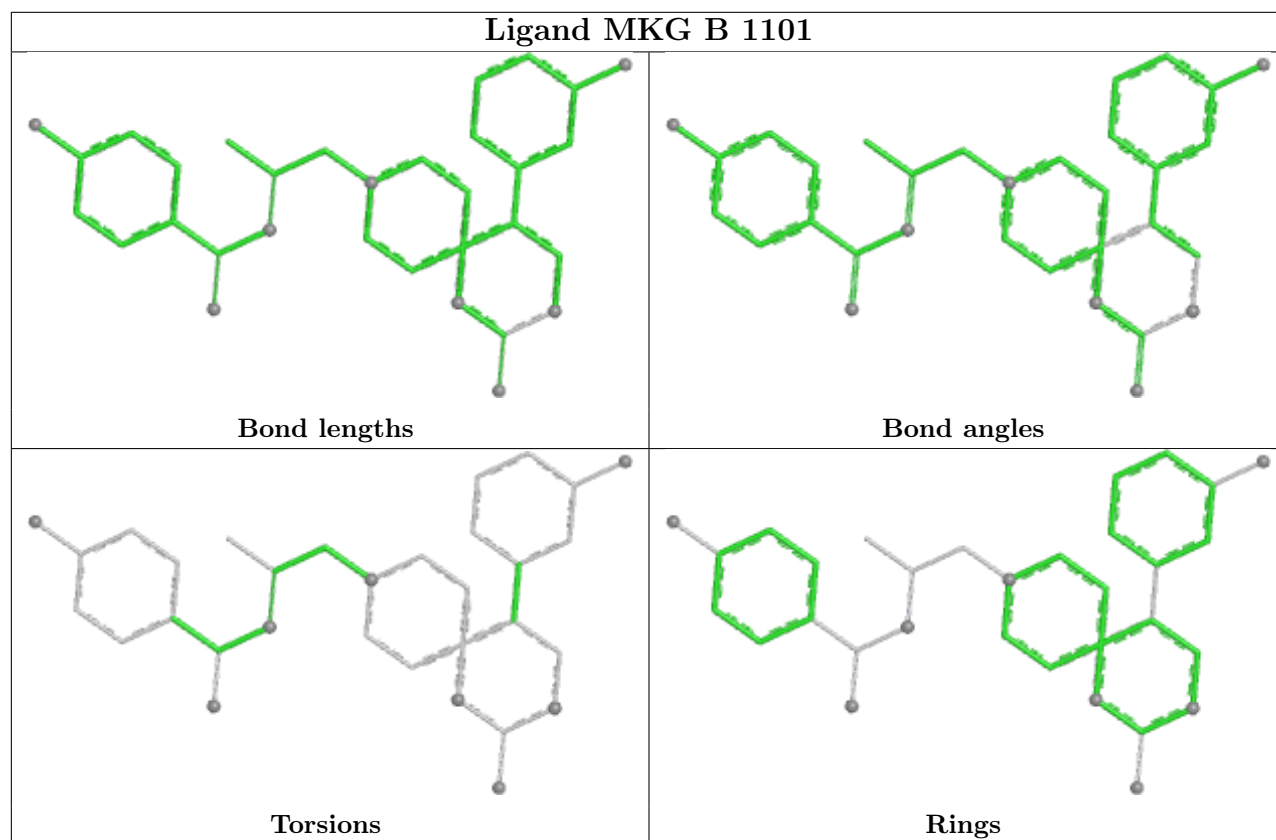
Ligand MKG D 1101

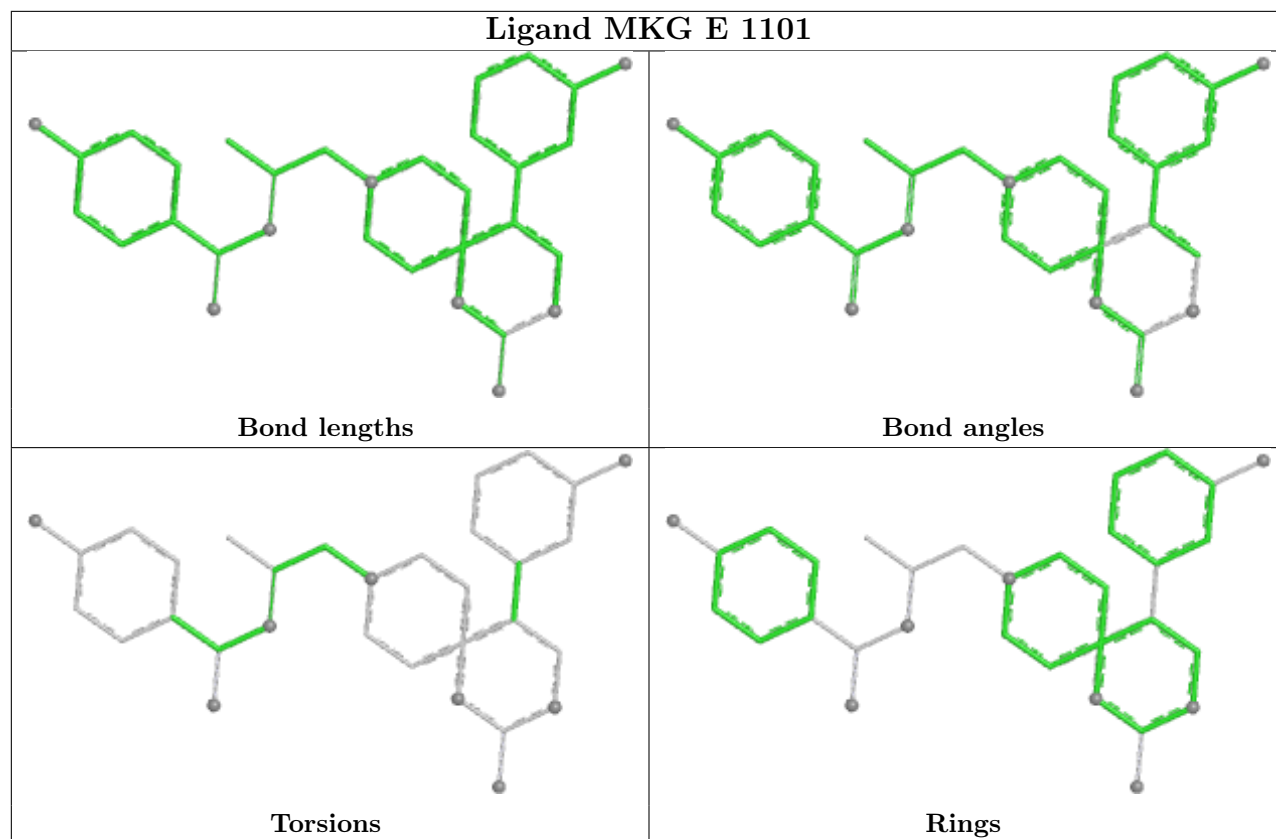


Ligand MKG A 1101



Ligand MKG B 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, 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	576/647 (89%)	-0.15	4 (0%) 84 69	27, 46, 76, 119	0
1	B	569/647 (87%)	-0.15	4 (0%) 84 69	26, 43, 72, 116	0
1	C	572/647 (88%)	-0.23	1 (0%) 91 85	25, 40, 67, 122	0
1	D	564/647 (87%)	-0.11	2 (0%) 88 79	28, 48, 77, 118	0
1	E	560/647 (86%)	0.55	20 (3%) 46 28	46, 83, 116, 179	0
1	F	526/647 (81%)	0.81	33 (6%) 26 17	60, 96, 139, 160	0
All	All	3367/3882 (86%)	0.11	64 (1%) 66 46	25, 53, 113, 179	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	681	LEU	4.4
1	F	974	ASN	3.6
1	F	781	VAL	3.6
1	E	612	CYS	3.6
1	C	673	TYR	3.0
1	F	854	LEU	3.0
1	F	850	LEU	2.9
1	F	697	PRO	2.9
1	F	871	ILE	2.8
1	F	883	GLY	2.8
1	E	374	GLU	2.8
1	E	415	ILE	2.8
1	B	394	VAL	2.7
1	F	490	ASN	2.7
1	B	682	LEU	2.7
1	F	896	THR	2.7
1	A	751	ASP	2.7
1	F	988	ALA	2.7
1	F	832	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	375	GLU	2.6
1	F	845	GLU	2.6
1	B	932	PRO	2.5
1	E	385	PRO	2.5
1	E	422	GLU	2.5
1	F	476	PHE	2.5
1	F	405	LEU	2.5
1	F	811	THR	2.5
1	E	445	ILE	2.4
1	E	644	ALA	2.4
1	F	341	GLY	2.4
1	E	680	PHE	2.4
1	E	402	ASP	2.4
1	F	337	ASP	2.4
1	F	648	HIS	2.4
1	E	663	TRP	2.3
1	E	467	LEU	2.3
1	E	1035	TRP	2.3
1	F	1036	THR	2.3
1	D	453	HIS	2.2
1	F	813	CYS	2.2
1	A	616	PHE	2.2
1	F	941	SER	2.2
1	F	1015	SER	2.2
1	F	921	CYS	2.2
1	F	773	GLU	2.2
1	D	932	PRO	2.2
1	F	750	ALA	2.2
1	A	935	ASP	2.2
1	F	1003	ARG	2.2
1	E	434	THR	2.2
1	E	607	HIS	2.2
1	B	848	GLY	2.2
1	F	758	LYS	2.1
1	E	337	ASP	2.1
1	F	938	ASP	2.1
1	F	491	GLU	2.1
1	F	836	SER	2.1
1	A	929	LEU	2.1
1	E	452	ASP	2.1
1	E	480	ILE	2.1
1	E	413	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	863	ILE	2.0
1	F	489	ASP	2.0
1	E	1029	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

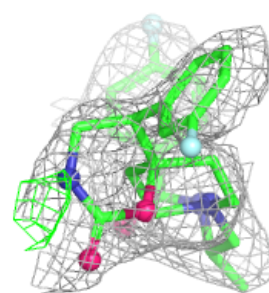
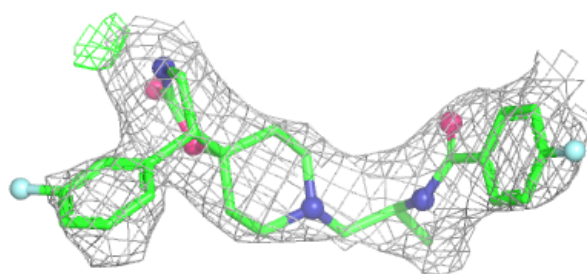
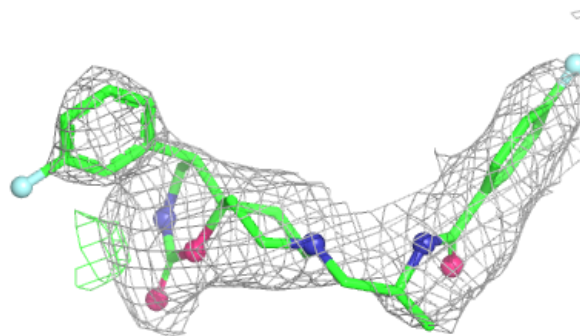
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MKG	F	1101	32/32	0.84	0.14	66,78,89,90	0
2	MKG	E	1101	32/32	0.88	0.14	67,74,89,92	0
2	MKG	B	1101	32/32	0.92	0.11	29,39,48,56	0
2	MKG	C	1101	32/32	0.92	0.11	31,38,46,60	0
2	MKG	D	1101	32/32	0.93	0.12	33,42,49,74	0
2	MKG	A	1101	32/32	0.94	0.10	34,43,57,71	0

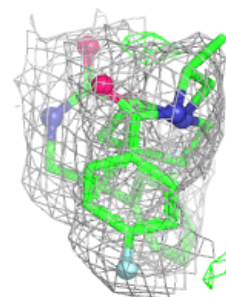
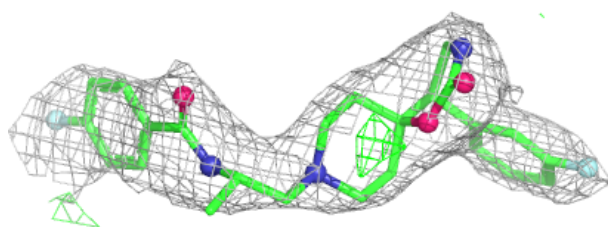
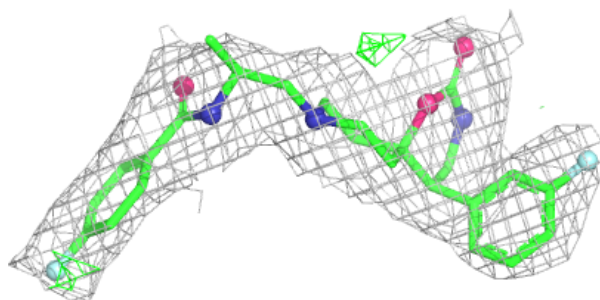
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MKG F 1101:

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

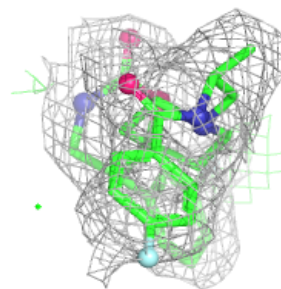
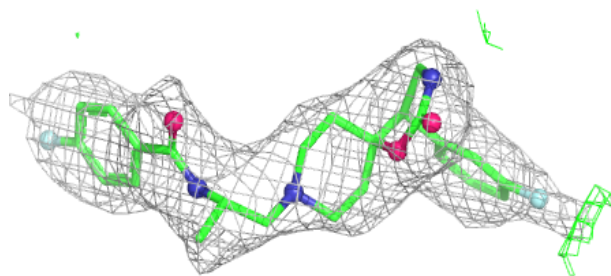
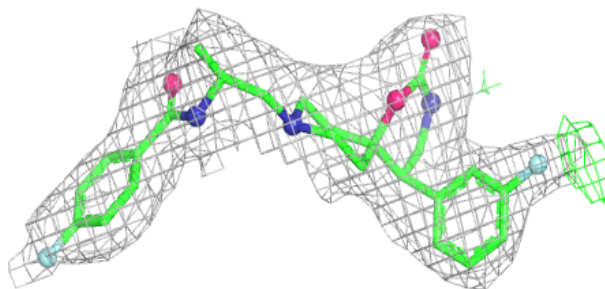
**Electron density around MKG E 1101:**

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

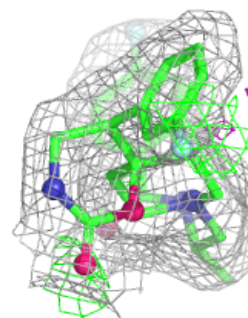
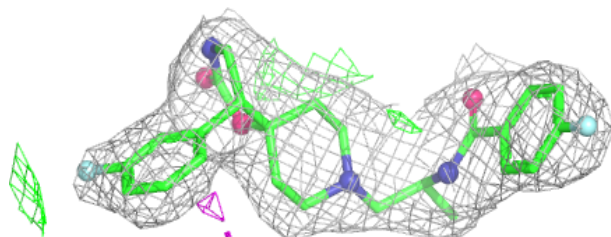
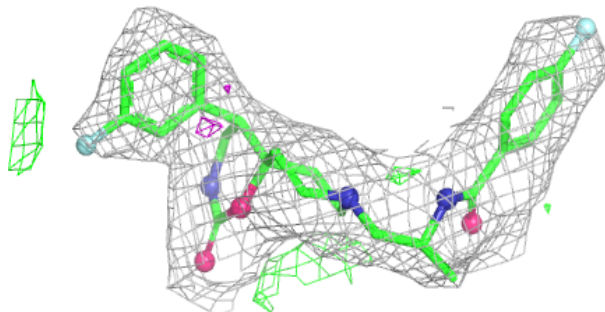


Electron density around MKG B 1101:

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

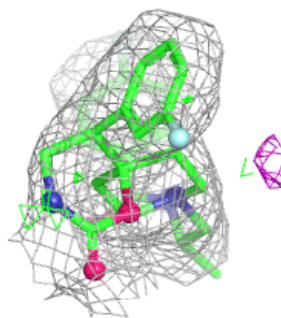
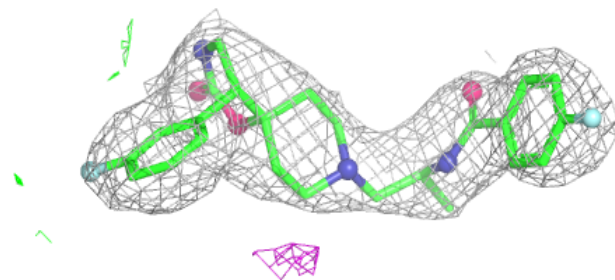
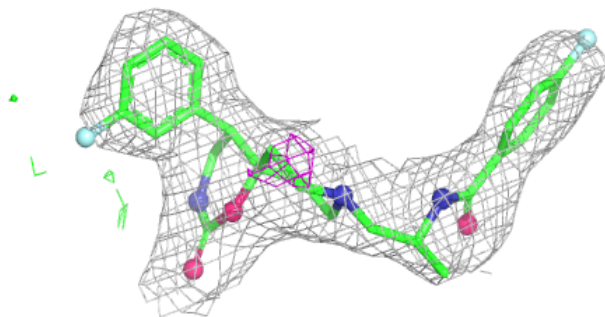
**Electron density around MKG C 1101:**

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

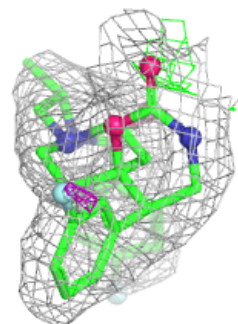
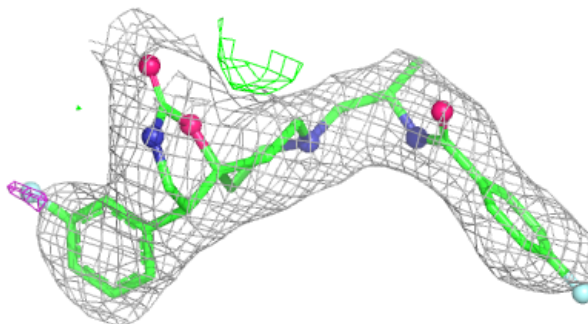


Electron density around MKG D 1101:

$2mF_o-DF_c$ (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.