



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:37 AM UTC

PDB ID : 8Z5E / pdb_00008z5e
Title : Crystal structure of beta-ketoacyl-ACP synthase FabF K336A in complex with octanoyl-ACP from *Helicobacter pylori*
Authors : Zhang, L.; Huang, Y.Z.
Deposited on : 2024-04-18
Resolution : 2.20 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

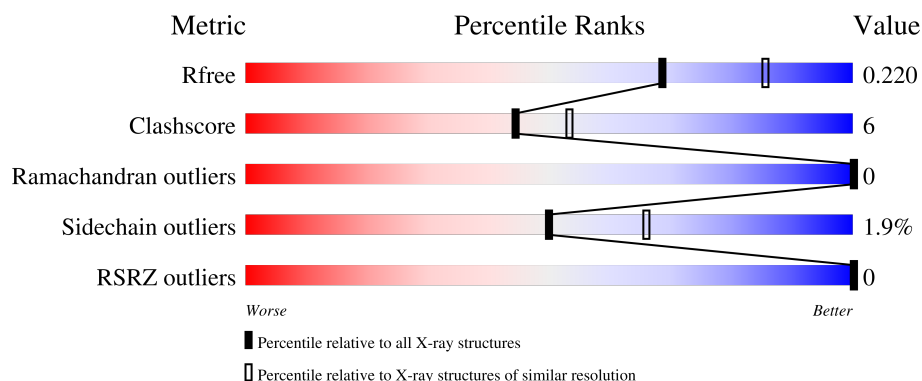
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	413	
1	B	413	
1	D	413	
1	E	413	
2	C	86	

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Mol	Chain	Length	Quality of chain
2	F	86	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (55%), yellow (35%), and orange (7%). The percentages are labeled below the bar.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14286 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 3-oxoacyl-[acyl-carrier-protein] synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3042	1910	525	585	22			
1	B	412	Total	C	N	O	S	0	1	0
			3050	1915	528	585	22			
1	D	412	Total	C	N	O	S	0	0	0
			3043	1910	525	586	22			
1	E	413	Total	C	N	O	S	0	0	0
			3049	1913	526	588	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A438WLJ1
A	336	ALA	LYS	engineered mutation	UNP A0A438WLJ1
B	0	SER	-	expression tag	UNP A0A438WLJ1
B	336	ALA	LYS	engineered mutation	UNP A0A438WLJ1
D	0	SER	-	expression tag	UNP A0A438WLJ1
D	336	ALA	LYS	engineered mutation	UNP A0A438WLJ1
E	0	SER	-	expression tag	UNP A0A438WLJ1
E	336	ALA	LYS	engineered mutation	UNP A0A438WLJ1

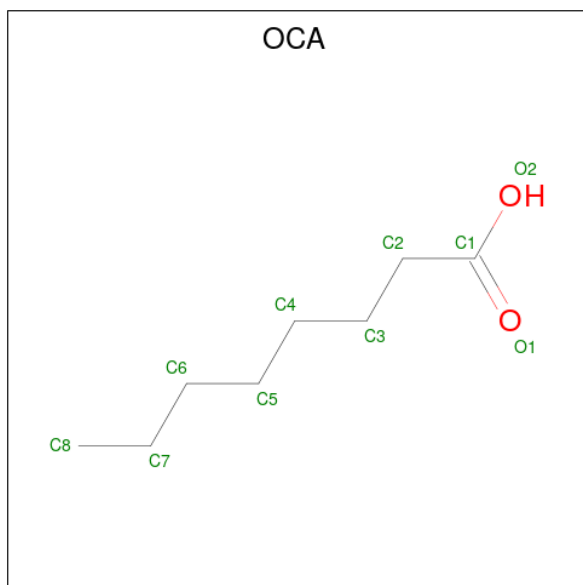
- Molecule 2 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	79	Total	C	N	O	S	0	0	0
			610	389	90	128	3			
2	F	80	Total	C	N	O	S	0	0	0
			615	392	91	129	3			

There are 16 discrepancies between the modelled and reference sequences:

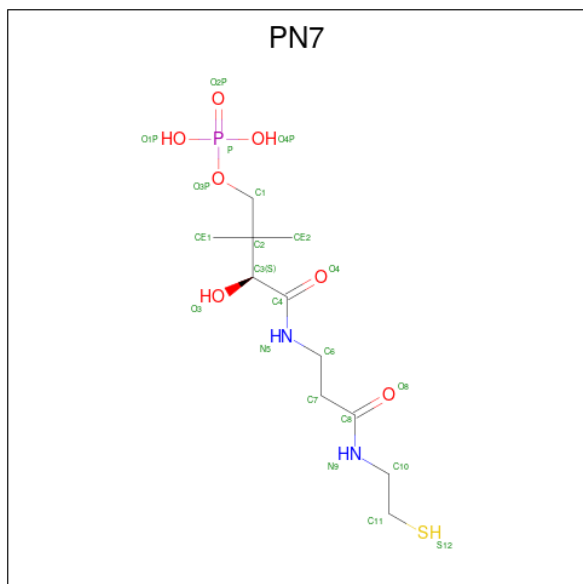
Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLY	-	expression tag	UNP Q5EDC8
C	-6	THR	-	expression tag	UNP Q5EDC8
C	-5	SER	-	expression tag	UNP Q5EDC8
C	-4	SER	-	expression tag	UNP Q5EDC8
C	-3	MET	-	expression tag	UNP Q5EDC8
C	-2	GLY	-	expression tag	UNP Q5EDC8
C	-1	TYR	-	expression tag	UNP Q5EDC8
C	0	LEU	-	expression tag	UNP Q5EDC8
F	-7	GLY	-	expression tag	UNP Q5EDC8
F	-6	THR	-	expression tag	UNP Q5EDC8
F	-5	SER	-	expression tag	UNP Q5EDC8
F	-4	SER	-	expression tag	UNP Q5EDC8
F	-3	MET	-	expression tag	UNP Q5EDC8
F	-2	GLY	-	expression tag	UNP Q5EDC8
F	-1	TYR	-	expression tag	UNP Q5EDC8
F	0	LEU	-	expression tag	UNP Q5EDC8

- Molecule 3 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: OCA) (formula: $C_8H_{16}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	8	1		
3	B	1	Total	C	O	0	0
			9	8	1		
3	D	1	Total	C	O	0	0
			9	8	1		
3	E	1	Total	C	O	0	0
			9	8	1		

- Molecule 4 is N 3 -[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-N-(2-sulfany ethyl)-beta-alaninamide (CCD ID: PN7) (formula: C₁₁H₂₃N₂O₇PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	F	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		

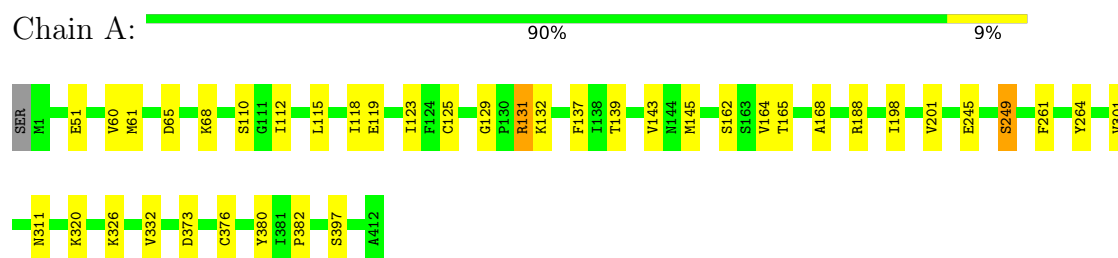
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	218	Total	O	0	0
			218	218		
5	B	171	Total	O	0	0
			171	171		
5	C	13	Total	O	0	0
			13	13		
5	D	217	Total	O	0	0
			217	217		
5	E	171	Total	O	0	0
			171	171		
5	F	9	Total	O	0	0
			9	9		

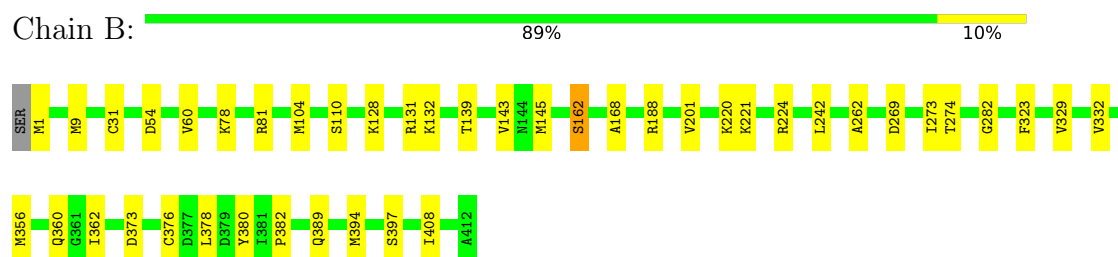
3 Residue-property plots

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

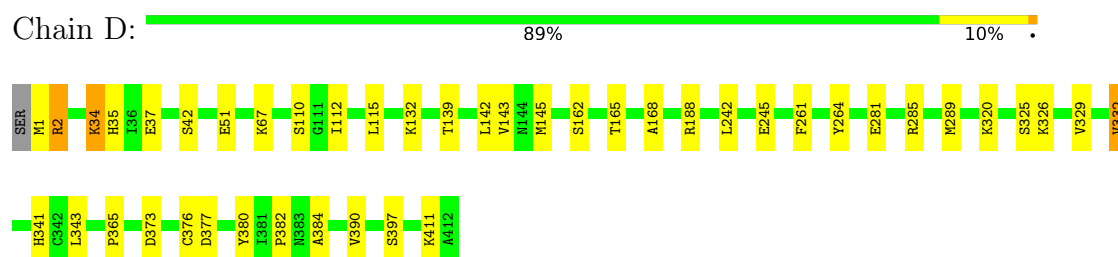
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 2



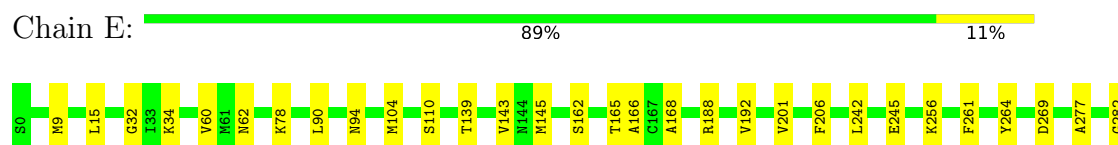
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 2



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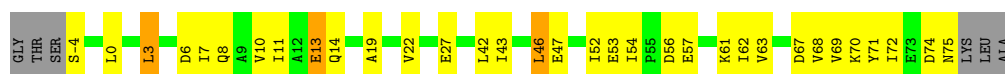




- Molecule 2: Acyl carrier protein



- Molecule 2: Acyl carrier protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.86Å 115.69Å 127.93Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	34.52 – 2.20 34.52 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.0 (34.52-2.20) 96.3 (34.52-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.62 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.164 , 0.213 0.174 , 0.220	Depositor DCC
R_{free} test set	4109 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.466 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14286	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OCA, PN7

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	0.47	0/3094	0.67	1/4170 (0.0%)
1	B	0.37	0/3105	0.58	1/4184 (0.0%)
1	D	0.41	0/3095	0.60	1/4170 (0.0%)
1	E	0.35	0/3101	0.56	1/4178 (0.0%)
2	C	0.62	0/616	0.92	1/835 (0.1%)
2	F	0.63	0/621	0.85	0/842
All	All	0.43	0/13632	0.63	5/18379 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	PRO	N-CA-C	6.37	121.27	110.95
1	B	382	PRO	N-CA-C	6.21	121.01	110.95
1	D	382	PRO	N-CA-C	6.11	120.03	110.80
1	E	382	PRO	N-CA-C	5.33	118.88	110.50
2	C	74	ASP	N-CA-C	-5.14	104.94	111.11

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain
1	D	2	ARG	Sidechain

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	3042	0	3043	23	0
1	B	3050	0	3056	27	0
1	D	3043	0	3043	29	0
1	E	3049	0	3048	26	0
2	C	610	0	600	28	0
2	F	615	0	602	27	0
3	A	9	0	15	0	0
3	B	9	0	15	0	0
3	D	9	0	15	0	0
3	E	9	0	15	3	0
4	C	21	0	22	3	0
4	F	21	0	22	2	0
5	A	218	0	0	0	0
5	B	171	0	0	0	0
5	C	13	0	0	1	0
5	D	217	0	0	3	0
5	E	171	0	0	0	0
5	F	9	0	0	0	0
All	All	14286	0	13496	162	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (162) 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:B:128:LYS:HE2	1:B:132:LYS:HG2	1.40	1.02
2:C:54:ILE:HG12	2:C:71:TYR:CE2	2.01	0.95
1:A:60:VAL:HG23	1:A:61:MET:HG3	1.71	0.72
1:D:110:SER:HB3	1:D:143:VAL:HG13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:GLU:HG2	2:F:63:VAL:HG22	1.72	0.70
2:C:67:ASP:O	2:C:70:LYS:HG3	1.92	0.68
2:F:74:ASP:O	2:F:75:ASN:C	2.37	0.67
4:C:101:PN7:S12	5:C:208:HOH:O	2.41	0.66
1:D:373:ASP:HB3	1:D:376:CYS:HB2	1.77	0.66
1:A:373:ASP:HB3	1:A:376:CYS:HB2	1.78	0.66
2:F:67:ASP:O	2:F:70:LYS:HG2	1.97	0.65
2:F:7:ILE:HD11	2:F:72:ILE:HD12	1.78	0.64
1:D:1:MET:CE	1:D:2:ARG:H	2.10	0.64
1:B:323:PHE:HD2	1:B:329:VAL:HG22	1.63	0.64
2:F:3:LEU:HD11	2:F:69:VAL:HG13	1.78	0.64
1:D:320:LYS:HZ2	1:D:326:LYS:H	1.46	0.63
1:B:9:MET:HG2	1:B:242:LEU:HD23	1.81	0.62
2:F:0:LEU:HA	2:F:3:LEU:HD23	1.81	0.62
2:F:8:GLN:NE2	2:F:22:VAL:HB	2.14	0.62
1:D:34:LYS:NZ	1:D:37:GLU:OE1	2.33	0.61
2:F:52:ILE:HD11	2:F:75:ASN:ND2	2.15	0.61
2:F:7:ILE:HG21	2:F:68:VAL:HG21	1.83	0.60
1:E:104:MET:HG3	1:E:188:ARG:HB2	1.85	0.59
2:F:54:ILE:HG12	2:F:71:TYR:CE2	2.36	0.59
2:C:52:ILE:HD12	2:C:72:ILE:HG23	1.85	0.58
1:D:1:MET:HG3	1:D:2:ARG:N	2.18	0.58
1:E:188:ARG:HG2	1:E:245:GLU:HG2	1.86	0.57
1:B:104:MET:HG3	1:B:188:ARG:HB2	1.87	0.57
1:B:60:VAL:HA	1:B:81:ARG:NH1	2.19	0.57
1:E:32:GLY:O	1:E:34:LYS:NZ	2.37	0.57
2:C:66:GLY:O	2:C:69:VAL:HG12	2.05	0.57
1:A:332:VAL:O	1:A:380:TYR:HA	2.05	0.56
2:F:8:GLN:NE2	2:F:19:ALA:O	2.39	0.56
2:C:8:GLN:HG3	2:C:22:VAL:CG1	2.36	0.56
1:A:261:PHE:HZ	1:A:264:TYR:HD2	1.53	0.55
1:E:206:PHE:HZ	3:E:501:OCA:H32	1.72	0.55
2:F:-4:SER:O	2:F:0:LEU:HG	2.07	0.55
2:F:43:ILE:HD11	2:F:62:ILE:HD12	1.88	0.55
2:C:52:ILE:HG22	2:C:53:GLU:H	1.71	0.54
1:E:301:VAL:HB	1:E:332:VAL:HG22	1.90	0.54
2:F:8:GLN:HA	2:F:22:VAL:HG11	1.89	0.54
1:D:34:LYS:HE3	1:D:35:HIS:O	2.08	0.54
1:A:65:ASP:HA	1:A:68:LYS:HE2	1.90	0.53
1:D:332:VAL:O	1:D:380:TYR:HA	2.08	0.53
1:A:311:ASN:HB2	4:C:101:PN7:C8	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:7:ILE:HG21	2:F:68:VAL:CG2	2.39	0.53
1:E:261:PHE:HZ	1:E:264:TYR:HD2	1.55	0.52
1:A:118:ILE:HA	1:A:137:PHE:CE1	2.45	0.52
1:D:289:MET:HE1	5:D:632:HOH:O	2.09	0.51
1:A:188:ARG:HG2	1:A:245:GLU:HG3	1.91	0.51
4:F:101:PN7:O4	4:F:101:PN7:H8	2.10	0.51
1:B:394:MET:HB2	1:B:408:ILE:HG12	1.93	0.51
1:E:360:GLN:HB3	1:E:362:ILE:HD12	1.93	0.51
2:F:0:LEU:O	2:F:3:LEU:HG	2.09	0.50
1:D:168:ALA:HA	1:D:397:SER:HB3	1.93	0.50
1:E:110:SER:HB3	1:E:143:VAL:HG13	1.94	0.50
2:C:7:ILE:O	2:C:11:ILE:HG13	2.12	0.50
2:F:14:GLN:HG3	2:F:42:LEU:HD23	1.94	0.49
2:C:71:TYR:CD2	2:C:71:TYR:C	2.89	0.49
2:F:7:ILE:O	2:F:11:ILE:HG13	2.12	0.49
2:C:68:VAL:O	2:C:72:ILE:HG12	2.12	0.49
1:D:42:SER:O	5:D:601:HOH:O	2.20	0.49
2:C:8:GLN:HG3	2:C:22:VAL:HG11	1.95	0.49
1:A:168:ALA:HA	1:A:397:SER:HB3	1.95	0.49
2:C:52:ILE:CD1	2:C:72:ILE:HG23	2.42	0.49
4:C:101:PN7:O4	4:C:101:PN7:H8	2.12	0.49
1:B:9:MET:HE1	1:B:356:MET:HG3	1.94	0.48
2:C:3:LEU:HD11	2:C:72:ILE:HG21	1.95	0.48
1:E:269:ASP:HB3	1:E:277:ALA:HB2	1.94	0.48
1:A:301:VAL:HB	1:A:332:VAL:HG22	1.95	0.48
2:F:13:GLU:OE1	2:F:14:GLN:HG2	2.13	0.48
1:D:1:MET:HE3	1:D:2:ARG:H	1.78	0.47
1:A:261:PHE:CZ	1:A:264:TYR:HD2	2.32	0.47
1:E:62:ASN:OD1	1:E:62:ASN:N	2.43	0.47
1:A:51:GLU:HG2	1:A:198:ILE:HD13	1.96	0.47
1:D:112:ILE:HD13	1:D:115:LEU:HD13	1.96	0.47
1:D:261:PHE:HZ	1:D:264:TYR:HD2	1.60	0.47
1:B:60:VAL:HG11	1:B:78:LYS:HA	1.97	0.47
1:B:221:LYS:O	1:B:224:ARG:HD2	2.15	0.47
1:E:269:ASP:OD1	1:E:282:GLY:HA3	2.14	0.47
1:A:320:LYS:HZ2	1:A:326:LYS:H	1.63	0.46
2:C:52:ILE:HG22	2:C:53:GLU:N	2.30	0.46
1:B:110:SER:HB3	1:B:143:VAL:HG13	1.98	0.46
1:B:54:ASP:OD1	1:B:54:ASP:N	2.48	0.46
1:B:269:ASP:OD1	1:B:282:GLY:HA3	2.15	0.46
1:A:139:THR:O	1:A:145:MET:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LYS:NZ	1:A:326:LYS:H	2.13	0.46
2:C:3:LEU:O	2:C:7:ILE:HG12	2.15	0.46
1:D:34:LYS:HE2	1:D:51:GLU:OE1	2.16	0.46
2:C:71:TYR:CD2	2:C:72:ILE:HD13	2.51	0.46
1:D:1:MET:HE2	1:D:2:ARG:H	1.79	0.46
1:E:389:GLN:NE2	1:E:389:GLN:HA	2.31	0.46
2:F:52:ILE:HG12	2:F:53:GLU:H	1.80	0.46
1:D:365:PRO:HB3	1:D:384:ALA:C	2.40	0.45
2:C:44:MET:O	2:C:48:GLU:HG3	2.17	0.45
1:B:31:CYS:HB3	1:B:220:LYS:HG3	1.97	0.45
1:E:343:LEU:HD22	3:E:501:OCA:H31	1.98	0.45
2:F:3:LEU:O	2:F:7:ILE:HG13	2.17	0.45
1:B:139:THR:O	1:B:145:MET:HG3	2.17	0.45
2:C:54:ILE:HG12	2:C:71:TYR:CZ	2.49	0.44
1:E:261:PHE:CZ	1:E:264:TYR:HD2	2.34	0.44
2:F:52:ILE:HD11	2:F:75:ASN:HD21	1.80	0.44
1:A:131:ARG:HE	1:A:132:LYS:HE2	1.82	0.44
1:B:273:ILE:HG13	1:B:274:THR:HG23	1.99	0.44
2:C:8:GLN:HG3	2:C:22:VAL:HG13	1.98	0.44
2:C:73:GLU:O	2:C:74:ASP:C	2.60	0.44
1:E:166:ALA:HB1	3:E:501:OCA:H41	1.99	0.44
1:B:1:MET:HE3	1:B:1:MET:HA	1.99	0.44
1:B:262:ALA:HB3	1:B:408:ILE:HG22	1.99	0.44
2:C:73:GLU:HG2	2:C:74:ASP:N	2.29	0.44
1:D:139:THR:O	1:D:145:MET:HG3	2.18	0.44
1:B:60:VAL:HA	1:B:81:ARG:HH12	1.83	0.44
1:A:118:ILE:HA	1:A:137:PHE:HE1	1.83	0.44
1:D:390:VAL:O	1:D:411:LYS:NZ	2.47	0.44
1:B:168:ALA:HA	1:B:397:SER:HB3	1.99	0.43
2:C:3:LEU:HD11	2:C:72:ILE:CG2	2.48	0.43
1:A:110:SER:HB3	1:A:143:VAL:HG13	2.01	0.43
1:A:112:ILE:HD13	1:A:115:LEU:HD13	2.00	0.43
2:F:52:ILE:CD1	2:F:75:ASN:HD21	2.30	0.43
1:B:323:PHE:CD2	1:B:329:VAL:HG22	2.48	0.43
2:C:30:LYS:HE2	2:C:31:ASP:OD1	2.18	0.43
1:D:188:ARG:HG2	1:D:245:GLU:HG3	2.01	0.43
1:E:168:ALA:HA	1:E:397:SER:HB3	2.01	0.43
1:D:377:ASP:OD1	5:D:602:HOH:O	2.22	0.42
1:E:380:TYR:O	1:E:381:ILE:C	2.62	0.42
1:B:332:VAL:O	1:B:380:TYR:HA	2.19	0.42
1:E:9:MET:HG2	1:E:242:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:ASP:HB3	1:E:376:CYS:HB2	2.01	0.42
1:D:320:LYS:NZ	1:D:326:LYS:H	2.14	0.42
2:F:57:GLU:O	2:F:61:LYS:HE3	2.19	0.42
2:C:54:ILE:CG1	2:C:71:TYR:CE2	2.90	0.42
1:D:341:HIS:NE2	1:D:343:LEU:HA	2.34	0.42
1:E:90:LEU:HB3	1:E:94:ASN:HA	2.02	0.42
1:D:261:PHE:CZ	1:D:264:TYR:HD2	2.37	0.41
1:E:60:VAL:HG11	1:E:78:LYS:HB2	2.03	0.41
1:B:131:ARG:NH2	2:C:47:GLU:OE1	2.54	0.41
1:B:389:GLN:NE2	1:B:389:GLN:HA	2.34	0.41
1:E:317:ILE:HA	1:E:320:LYS:HE2	2.02	0.41
2:C:18:ASP:HB3	2:C:20:ALA:H	1.85	0.41
1:D:341:HIS:CD2	1:D:343:LEU:HD23	2.55	0.41
1:E:15:LEU:HD23	1:E:15:LEU:HA	1.93	0.41
1:A:125:CYS:HA	1:A:129:GLY:O	2.20	0.41
2:C:57:GLU:HA	2:C:60:GLU:HG3	2.03	0.41
2:C:71:TYR:HA	2:C:74:ASP:OD2	2.21	0.41
2:C:18:ASP:HB2	2:C:21:GLN:HE22	1.86	0.41
1:D:67:LYS:HA	1:D:67:LYS:HD3	1.91	0.41
1:D:142:LEU:HB2	1:D:145:MET:HG2	2.03	0.41
1:E:9:MET:HG2	1:E:242:LEU:HD23	2.02	0.41
1:E:332:VAL:O	1:E:380:TYR:HA	2.21	0.41
2:F:46:LEU:HD12	2:F:46:LEU:HA	1.95	0.41
4:F:101:PN7:H17	4:F:101:PN7:H13	1.63	0.41
1:A:119:GLU:O	1:A:123:ILE:HG13	2.20	0.41
1:A:164:VAL:HG12	1:B:162:SER:HB3	2.03	0.40
1:D:281:GLU:CD	1:D:285:ARG:HE	2.30	0.40
1:B:373:ASP:HB3	1:B:376:CYS:HB2	2.03	0.40
1:D:325:SER:O	1:D:329:VAL:HG23	2.21	0.40
1:E:139:THR:O	1:E:145:MET:HG3	2.22	0.40
2:F:6:ASP:O	2:F:10:VAL:HG23	2.20	0.40
1:B:360:GLN:HB3	1:B:362:ILE:HD12	2.03	0.40
1:A:188:ARG:NH2	1:A:249:SER:OG	2.55	0.40
1:B:378:LEU:HB2	1:B:380:TYR:CE1	2.56	0.40
2:F:47:GLU:HA	2:F:52:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

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	410/413 (99%)	395 (96%)	15 (4%)	0	100	100
1	B	411/413 (100%)	396 (96%)	15 (4%)	0	100	100
1	D	410/413 (99%)	391 (95%)	19 (5%)	0	100	100
1	E	411/413 (100%)	392 (95%)	19 (5%)	0	100	100
2	C	77/86 (90%)	74 (96%)	3 (4%)	0	100	100
2	F	78/86 (91%)	74 (95%)	4 (5%)	0	100	100
All	All	1797/1824 (98%)	1722 (96%)	75 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	317/318 (100%)	313 (99%)	4 (1%)	61	76
1	B	318/318 (100%)	316 (99%)	2 (1%)	78	89
1	D	317/318 (100%)	311 (98%)	6 (2%)	50	66
1	E	318/318 (100%)	312 (98%)	6 (2%)	50	66
2	C	66/71 (93%)	61 (92%)	5 (8%)	12	14
2	F	66/71 (93%)	62 (94%)	4 (6%)	17	20
All	All	1402/1414 (99%)	1375 (98%)	27 (2%)	50	66

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	SER
1	A	165	THR
1	A	201	VAL
1	A	249	SER
1	B	162	SER
1	B	201	VAL
2	C	0	LEU
2	C	65	VAL
2	C	70	LYS
2	C	73	GLU
2	C	75	ASN
1	D	34	LYS
1	D	132	LYS
1	D	162	SER
1	D	165	THR
1	D	242	LEU
1	D	332	VAL
1	E	162	SER
1	E	165	THR
1	E	192	VAL
1	E	201	VAL
1	E	256	LYS
1	E	322	VAL
2	F	3	LEU
2	F	13	GLU
2	F	46	LEU
2	F	56	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	102	ASN
1	B	35	HIS
1	B	117	ASN
1	B	271	ASN
1	B	302	ASN
1	B	309	HIS
1	B	404	ASN
2	C	75	ASN
1	D	74	GLN

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Mol	Chain	Res	Type
1	D	309	HIS
1	D	404	ASN
1	E	359	ASN
1	E	389	GLN
1	E	404	ASN
2	F	8	GLN
2	F	75	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	OCA	E	501	1	7,8,9	0.15	0	6,7,9	0.30	0
3	OCA	A	501	1	7,8,9	0.14	0	6,7,9	0.15	0
4	PN7	F	101	2	14,20,21	0.57	0	18,26,29	2.34	6 (33%)
3	OCA	B	501	1	7,8,9	0.15	0	6,7,9	0.21	0
3	OCA	D	501	1	7,8,9	0.16	0	6,7,9	0.22	0
4	PN7	C	101	2	14,20,21	0.53	0	18,26,29	2.72	6 (33%)

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
3	OCA	E	501	1	-	3/6/6/7	-
3	OCA	A	501	1	-	3/6/6/7	-
4	PN7	F	101	2	-	15/24/26/27	-
3	OCA	B	501	1	-	4/6/6/7	-
3	OCA	D	501	1	-	4/6/6/7	-
4	PN7	C	101	2	-	10/24/26/27	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	101	PN7	C6-N5-C4	7.36	135.76	122.55
4	F	101	PN7	C6-N5-C4	6.68	134.54	122.55
4	C	101	PN7	C6-C7-C8	-5.77	102.78	112.39
4	F	101	PN7	CE2-C2-C3	3.79	115.22	108.77
4	C	101	PN7	CE2-C2-C3	3.14	114.12	108.77
4	F	101	PN7	C10-N9-C8	3.09	128.57	122.82
4	C	101	PN7	C3-C4-N5	-3.06	110.68	116.48
4	C	101	PN7	C11-C10-N9	-3.06	105.37	112.31
4	F	101	PN7	C11-C10-N9	-3.03	105.42	112.31
4	C	101	PN7	C10-N9-C8	2.93	128.27	122.82
4	F	101	PN7	C3-C4-N5	-2.48	111.78	116.48
4	F	101	PN7	C6-C7-C8	-2.00	109.06	112.39

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	OCA	O1-C1-C2-C3
3	B	501	OCA	O1-C1-C2-C3
3	D	501	OCA	O1-C1-C2-C3
4	C	101	PN7	O3P-C1-C2-CE1
4	C	101	PN7	O3P-C1-C2-CE2
4	C	101	PN7	O3P-C1-C2-C3
4	F	101	PN7	O3P-C1-C2-CE1
4	F	101	PN7	O3P-C1-C2-CE2

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Mol	Chain	Res	Type	Atoms
4	F	101	PN7	O3P-C1-C2-C3
4	F	101	PN7	C1-C2-C3-O3
4	F	101	PN7	C1-C2-C3-C4
4	F	101	PN7	CE2-C2-C3-O3
4	F	101	PN7	CE2-C2-C3-C4
4	F	101	PN7	O3-C3-C4-O4
4	F	101	PN7	O3-C3-C4-N5
4	F	101	PN7	N5-C6-C7-C8
4	F	101	PN7	C7-C6-N5-C4
4	C	101	PN7	C7-C6-N5-C4
3	A	501	OCA	C2-C3-C4-C5
3	E	501	OCA	C3-C4-C5-C6
3	E	501	OCA	C4-C5-C6-C7
3	D	501	OCA	C3-C4-C5-C6
4	C	101	PN7	O3-C3-C4-O4
4	C	101	PN7	C6-C7-C8-O8
4	F	101	PN7	CE1-C2-C3-O3
3	E	501	OCA	C2-C3-C4-C5
4	C	101	PN7	C2-C3-C4-O4
4	F	101	PN7	C2-C3-C4-O4
4	C	101	PN7	C2-C3-C4-N5
4	F	101	PN7	C2-C3-C4-N5
3	B	501	OCA	C3-C4-C5-C6
4	F	101	PN7	CE1-C2-C3-C4
3	A	501	OCA	C1-C2-C3-C4
3	D	501	OCA	C5-C6-C7-C8
4	C	101	PN7	C6-C7-C8-N9
3	B	501	OCA	C4-C5-C6-C7
3	B	501	OCA	C1-C2-C3-C4
3	D	501	OCA	C1-C2-C3-C4
4	C	101	PN7	O3-C3-C4-N5

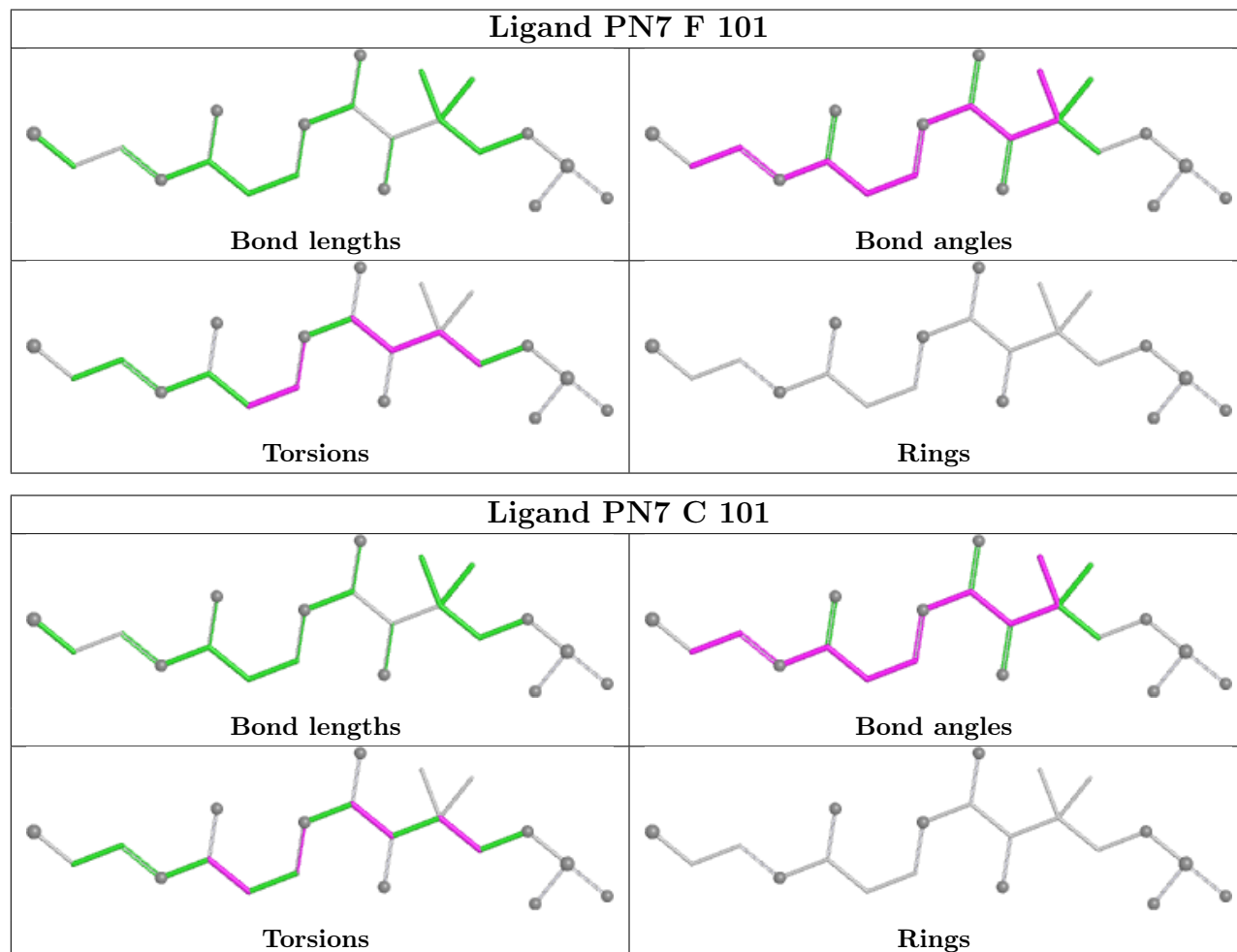
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	OCA	3	0
4	F	101	PN7	2	0
4	C	101	PN7	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	412/413 (99%)	-1.44	0 100 100	15, 24, 38, 54	0
1	B	412/413 (99%)	-1.35	0 100 100	16, 29, 44, 57	1 (0%)
1	D	412/413 (99%)	-1.38	0 100 100	16, 24, 39, 54	0
1	E	413/413 (100%)	-1.34	0 100 100	18, 30, 45, 64	0
2	C	79/86 (91%)	-0.58	0 100 100	33, 90, 145, 173	0
2	F	80/86 (93%)	-0.53	0 100 100	37, 99, 148, 187	0
All	All	1808/1824 (99%)	-1.31	0 100 100	15, 28, 90, 187	1 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
4	PN7	F	101	21/22	0.98	0.04	30,36,44,51	0

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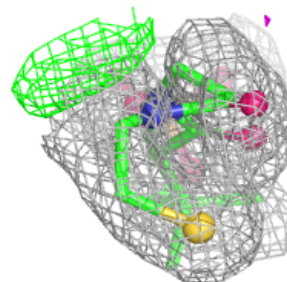
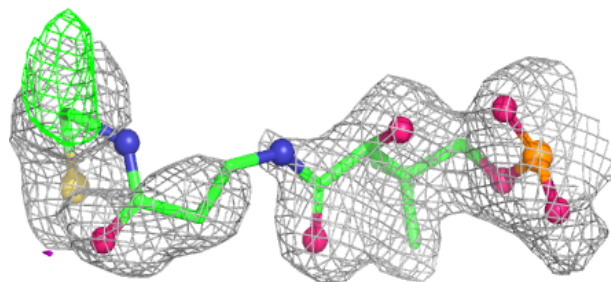
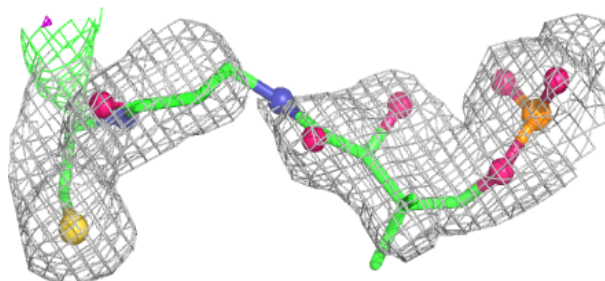
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OCA	B	501	9/10	0.99	0.05	21,22,25,33	0
3	OCA	D	501	9/10	0.99	0.05	19,20,23,24	0
3	OCA	E	501	9/10	0.99	0.04	21,23,28,28	0
4	PN7	C	101	21/22	0.99	0.03	28,32,40,42	0
3	OCA	A	501	9/10	0.99	0.04	19,20,26,28	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.

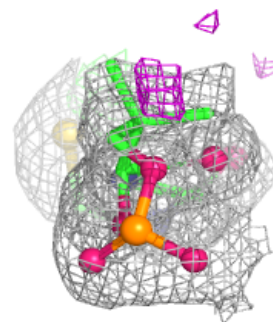
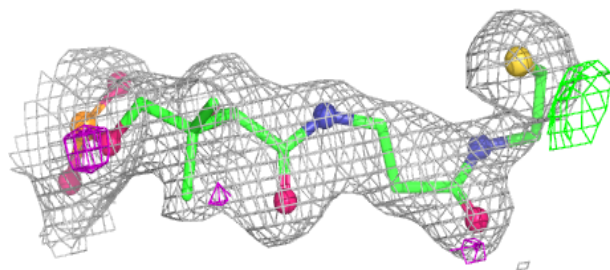
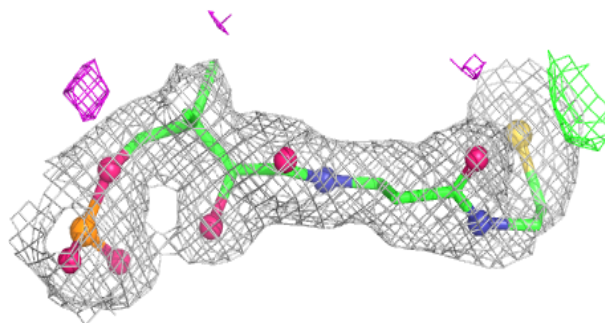
Electron density around PN7 F 101:

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 PN7 C 101:

$2mF_o-DF_c$ (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.