

wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2023 – 03:21 AM EDT

PDB ID : 5WKC

Title : Saccharomyces cerevisiae acetohydroxyacid synthase in complex with the her-

bicide penoxsulam

Authors: Guddat, W.L.; Lonhienne, G.T.

Deposited on : 2017-07-25

Resolution : 2.33 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) 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 : 2.35.1

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

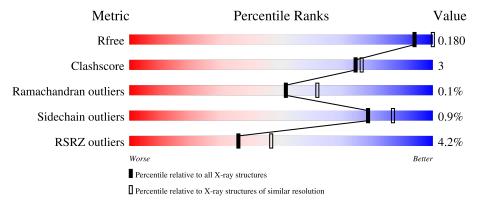
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.33 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	A	677	82%	5%	13%
1	В	677	82%	6%	12%
1	Е	677	80%	7%	13%
2	D	677	82%	5%	12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	F50	A	704	-	-	X	-
6	F50	В	705	-	-	X	-
6	F50	E	705	-	-	X	-



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 19824 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 Acetolactate synthase catalytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	۸	A 591	Total	С	N	О	S	0	0 3	0
1	A		4526	2866	784	854	22	0		
1	В	598	Total	С	N	О	S	0	4	0
1	Б	990	4580	2898	792	868	22	0		
1	Е	502	Total	С	N	О	S	0	2	0
1		592	4528	2868	782	856	22	U	2	

There are 141 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	UNP P07342
A	12	HIS	-	expression tag	UNP P07342
A	13	HIS	-	expression tag	UNP P07342
A	14	HIS	-	expression tag	UNP P07342
A	15	HIS	-	expression tag	UNP P07342
A	16	HIS	-	expression tag	UNP P07342
A	17	HIS	-	expression tag	UNP P07342
A	18	SER	-	expression tag	UNP P07342
A	19	SER	-	expression tag	UNP P07342
A	20	GLY	-	expression tag	UNP P07342
A	21	LEU	-	expression tag	UNP P07342
A	22	VAL	-	expression tag	UNP P07342
A	23	PRO	-	expression tag	UNP P07342
A	24	ARG	-	expression tag	UNP P07342
A	25	GLY	-	expression tag	UNP P07342
A	26	SER	-	expression tag	UNP P07342
A	27	GLY	-	expression tag	UNP P07342
A	28	MET	-	expression tag	UNP P07342
A	29	LYS		expression tag	UNP P07342
A	30	GLU	-	expression tag	UNP P07342
A	31	THR	-	expression tag	UNP P07342
A	32	ALA	-	expression tag	UNP P07342
A	33	ALA	_	expression tag	UNP P07342



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Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ALA	-	expression tag	UNP P07342
A	35	LYS	-	expression tag	UNP P07342
A	36	PHE	-	expression tag	UNP P07342
A	37	GLU	-	expression tag	UNP P07342
A	38	ARG	-	expression tag	UNP P07342
A	39	GLN	-	expression tag	UNP P07342
A	40	HIS	-	expression tag	UNP P07342
A	41	MET	-	expression tag	UNP P07342
A	42	ASP	-	expression tag	UNP P07342
A	43	SER	-	expression tag	UNP P07342
A	44	PRO	-	expression tag	UNP P07342
A	45	ASP	-	expression tag	UNP P07342
A	46	LEU	-	expression tag	UNP P07342
A	47	GLY	-	expression tag	UNP P07342
A	48	THR	-	expression tag	UNP P07342
A	49	ASP	-	expression tag	UNP P07342
A	50	ASP	-	expression tag	UNP P07342
A	51	ASP	-	expression tag	UNP P07342
A	52	ASP	-	expression tag	UNP P07342
A	53	LYS	-	expression tag	UNP P07342
A	54	ALA	-	expression tag	UNP P07342
A	55	MET	-	expression tag	UNP P07342
A	56	GLY	-	expression tag	UNP P07342
A	57	SER	-	expression tag	UNP P07342
В	11	MET	-	initiating methionine	UNP P07342
В	12	HIS	-	expression tag	UNP P07342
В	13	HIS	-	expression tag	UNP P07342
В	14	HIS	-	expression tag	UNP P07342
В	15	HIS	-	expression tag	UNP P07342
В	16	HIS	-	expression tag	UNP P07342
В	17	HIS	-	expression tag	UNP P07342
В	18	SER	-	expression tag	UNP P07342
В	19	SER	-	expression tag	UNP P07342
В	20	GLY	-	expression tag	UNP P07342
В	21	LEU	-	expression tag	UNP P07342
В	22	VAL	-	expression tag	UNP P07342
В	23	PRO	-	expression tag	UNP P07342
В	24	ARG	-	expression tag	UNP P07342
В	25	GLY	-	expression tag	UNP P07342
В	26	SER	-	expression tag	UNP P07342
В	27	GLY	-	expression tag	UNP P07342
В	28	MET	-	expression tag	UNP P07342



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Chain	Residue	Modelled	Actual	Comment	Reference
В	29	LYS	_	expression tag	UNP P07342
В	30	GLU	_	expression tag	UNP P07342
В	31	THR	_	expression tag	UNP P07342
В	32	ALA	_	expression tag	UNP P07342
В	33	ALA	_	expression tag	UNP P07342
В	34	ALA	_	expression tag	UNP P07342
В	35	LYS	_	expression tag	UNP P07342
В	36	PHE	_	expression tag	UNP P07342
В	37	GLU	_	expression tag	UNP P07342
В	38	ARG	-	expression tag	UNP P07342
В	39	GLN	-	expression tag	UNP P07342
В	40	HIS	-	expression tag	UNP P07342
В	41	MET	-	expression tag	UNP P07342
В	42	ASP	-	expression tag	UNP P07342
В	43	SER	-	expression tag	UNP P07342
В	44	PRO	_	expression tag	UNP P07342
В	45	ASP	_	expression tag	UNP P07342
В	46	LEU	-	expression tag	UNP P07342
В	47	GLY	_	expression tag	UNP P07342
В	48	THR	-	expression tag	UNP P07342
В	49	ASP	-	expression tag	UNP P07342
В	50	ASP	-	expression tag	UNP P07342
В	51	ASP	-	expression tag	UNP P07342
В	52	ASP	-	expression tag	UNP P07342
В	53	LYS	-	expression tag	UNP P07342
В	54	ALA	-	expression tag	UNP P07342
В	55	MET	-	expression tag	UNP P07342
В	56	GLY	-	expression tag	UNP P07342
В	57	SER	_	expression tag	UNP P07342
Е	11	MET	_	initiating methionine	UNP P07342
Е	12	HIS	-	expression tag	UNP P07342
Е	13	HIS	-	expression tag	UNP P07342
Е	14	HIS	-	expression tag	UNP P07342
Е	15	HIS	-	expression tag	UNP P07342
Е	16	HIS	-	expression tag	UNP P07342
Е	17	HIS	-	expression tag	UNP P07342
Е	18	SER	-	expression tag	UNP P07342
Е	19	SER	-	expression tag	UNP P07342
Е	20	GLY	-	expression tag	UNP P07342
E	21	LEU	-	expression tag	UNP P07342
E	22	VAL	-	expression tag	UNP P07342
Е	23	PRO	-	expression tag	UNP P07342



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Chain	Residue	Modelled	Actual	Comment	Reference
Е	24	ARG	-	expression tag	UNP P07342
Е	25	GLY	-	expression tag	UNP P07342
Е	26	SER	-	expression tag	UNP P07342
E	27	GLY	-	expression tag	UNP P07342
Е	28	MET	-	expression tag	UNP P07342
E	29	LYS	_	expression tag	UNP P07342
E	30	GLU	-	expression tag	UNP P07342
Е	31	THR	-	expression tag	UNP P07342
E	32	ALA	-	expression tag	UNP P07342
Е	33	ALA	-	expression tag	UNP P07342
Е	34	ALA	-	expression tag	UNP P07342
Е	35	LYS	-	expression tag	UNP P07342
Е	36	PHE	-	expression tag	UNP P07342
E	37	GLU	-	expression tag	UNP P07342
Е	38	ARG	-	expression tag	UNP P07342
E	39	GLN	-	expression tag	UNP P07342
Е	40	HIS	-	expression tag	UNP P07342
Е	41	MET	-	expression tag	UNP P07342
Е	42	ASP	-	expression tag	UNP P07342
Е	43	SER	-	expression tag	UNP P07342
Е	44	PRO	-	expression tag	UNP P07342
Е	45	ASP	-	expression tag	UNP P07342
Е	46	LEU	-	expression tag	UNP P07342
Е	47	GLY	-	expression tag	UNP P07342
Е	48	THR	-	expression tag	UNP P07342
Е	49	ASP	-	expression tag	UNP P07342
Е	50	ASP	-	expression tag	UNP P07342
Е	51	ASP	-	expression tag	UNP P07342
Е	52	ASP	-	expression tag	UNP P07342
Е	53	LYS	-	expression tag	UNP P07342
Е	54	ALA	-	expression tag	UNP P07342
Е	55	MET	-	expression tag	UNP P07342
Е	56	GLY	-	expression tag	UNP P07342
Е	57	SER	-	expression tag	UNP P07342

• Molecule 2 is a protein called Acetolactate synthase catalytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	D	596	Total	С	N	О	S	0	1	0
	ט	390	4553	2880	789	862	22	0	1	U

There are 47 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
D	11	MET	-	initiating methionine	UNP P07342
D	12	HIS	-	expression tag	UNP P07342
D	13	HIS	-	expression tag	UNP P07342
D	14	HIS	-	expression tag	UNP P07342
D	15	HIS	-	expression tag	UNP P07342
D	16	HIS	-	expression tag	UNP P07342
D	17	HIS	-	expression tag	UNP P07342
D	18	SER	-	expression tag	UNP P07342
D	19	SER	-	expression tag	UNP P07342
D	20	GLY	-	expression tag	UNP P07342
D	21	LEU	-	expression tag	UNP P07342
D	22	VAL	-	expression tag	UNP P07342
D	23	PRO	-	expression tag	UNP P07342
D	24	ARG	-	expression tag	UNP P07342
D	25	GLY	-	expression tag	UNP P07342
D	26	SER	-	expression tag	UNP P07342
D	27	GLY	-	expression tag	UNP P07342
D	28	MET	-	expression tag	UNP P07342
D	29	LYS	-	expression tag	UNP P07342
D	30	GLU	-	expression tag	UNP P07342
D	31	THR	-	expression tag	UNP P07342
D	32	ALA	-	expression tag	UNP P07342
D	33	ALA	-	expression tag	UNP P07342
D	34	ALA	-	expression tag	UNP P07342
D	35	LYS	-	expression tag	UNP P07342
D	36	PHE	-	expression tag	UNP P07342
D	37	GLU	-	expression tag	UNP P07342
D	38	ARG	-	expression tag	UNP P07342
D	39	GLN	-	expression tag	UNP P07342
D	40	HIS	-	expression tag	UNP P07342
D	41	MET	-	expression tag	UNP P07342
D	42	ASP	-	expression tag	UNP P07342
D	43	SER	-	expression tag	UNP P07342
D	44	PRO	-	expression tag	UNP P07342
D	45	ASP	-	expression tag	UNP P07342
D	46	LEU	-	expression tag	UNP P07342
D	47	GLY	-	expression tag	UNP P07342
D	48	THR	-	expression tag	UNP P07342
D	49	ASP	-	expression tag	UNP P07342
D	50	ASP	-	expression tag	UNP P07342
D	51	ASP	-	expression tag	UNP P07342
D	52	ASP	-	expression tag	UNP P07342
D	53	LYS	-	expression tag	UNP P07342



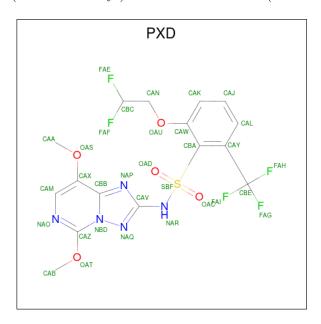
Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Chain	Residue	Modelled	Actual	Comment	Reference
D	54	ALA	-	expression tag	UNP P07342
D	55	MET	-	expression tag	UNP P07342
D	56	GLY	-	expression tag	UNP P07342
D	57	SER	-	expression tag	UNP P07342

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	В	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

• Molecule 4 is 2-(2,2-difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide (three-letter code: PXD) (formula: $C_{16}H_{14}F_5N_5O_5S$).



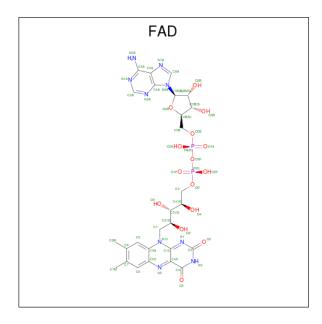
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
1	A	1	Total	С	F	N	О	S	0	0
-1	11	1	32	16	5	5	5	1	0	U
1	R	1	Total	С	F	N	Ο	S	0	0
4	Ъ	1	32	16	5	5	5	1	0	U
1	Е	1	Total	С	F	N	О	S	0	0
4	12	1	32	16	5	5	5	1	0	U



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	D	1	Total 32	C 16	F 5	N 5	O 5	S 1	0	0

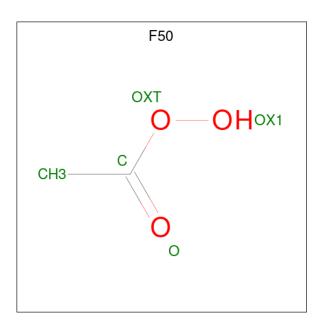
• Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	Λ	1	Total	С	N	О	Р	0	0
	Λ	1	53	27	9	15	2	U	0
5	R	1	Total	С	N	О	Р	0	0
9	Б	1	53	27	9	15	2	U	
5	E	1	Total	С	N	О	Р	0	0
9	تا ا	1	53	27	9	15	2	U	0
5	D	1	Total	С	N	О	Р	0	0
	ש	1	53	27	9	15	2	U	U

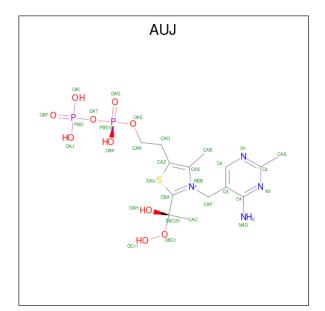
 \bullet Molecule 6 is ETHANEPEROXOIC ACID (three-letter code: F50) (formula: $\mathrm{C_2H_4O_3}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 5 2 3	0	0
6	В	1	Total C O 5 2 3	0	0
6	E	1	Total C O 5 2 3	0	0

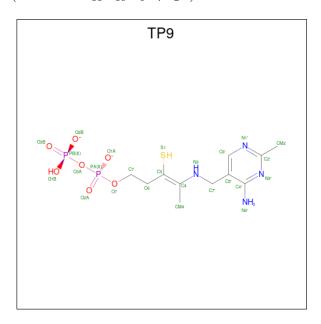
• Molecule 7 is 2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-2-[(1 $\{S\}$)-1-(dioxidanyl)-1-oxidanyl-ethyl]-4-methyl-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (three-letter code: AUJ) (formula: $C_{14}H_{23}N_4O_{10}P_2S$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	Δ	1	Total	С	N	О	Р	S	0	0
'	11	1	31	14	4	10	2	1		

• Molecule 8 is (3Z)-4-{[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]AMINO}-3-M ERCAPTOPENT-3-EN-1-YL TRIHYDROGEN DIPHOSPHATE (three-letter code: TP9) (formula: $C_{11}H_{18}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
8	В	1	Total 25		N 4				0	0
8	Е	1	Total 25		N 4				0	0
8	D	1	Total 25		N 4			S 1	0	0

• Molecule 9 is water.

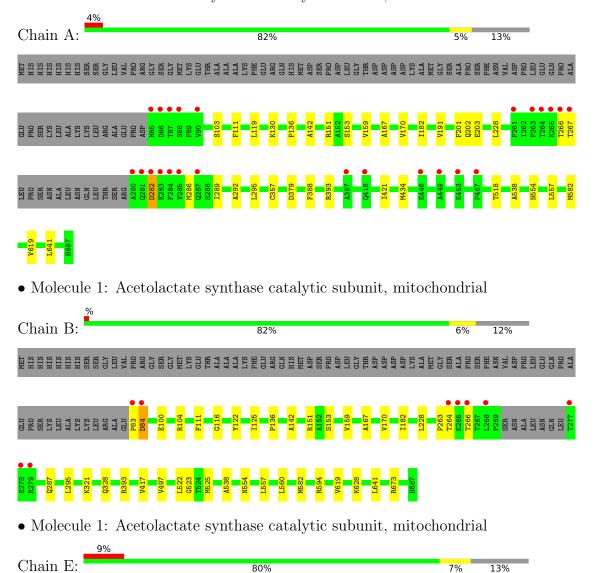
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	260	Total O 260 260	0	0
9	В	357	Total O 357 357	0	0
9	E	177	Total O 177 177	0	0
9	D	378	Total O 378 378	0	0



3 Residue-property plots (i)

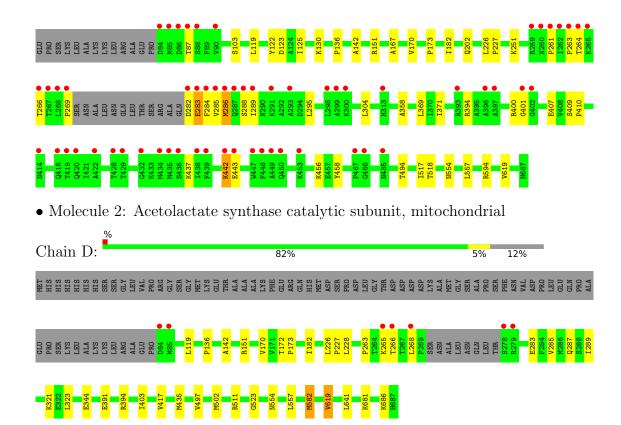
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial



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4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants	218.21Å 218.21Å 361.94Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 - 2.33	Depositor
Resolution (A)	48.79 - 2.33	EDS
% Data completeness	99.9 (48.79-2.33)	Depositor
(in resolution range)	99.9 (48.79-2.33)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.54 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
D.D.	0.150 , 0.180	Depositor
R, R_{free}	0.156 , 0.180	DCC
R_{free} test set	2000 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 52.7	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19824	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: SME, AUJ, PXD, TP9, FAD, MG, F50

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).

Mal	Mol Chain		lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.35	0/4630	0.44	0/6276	
1	В	0.34	0/4688	0.46	0/6356	
1	Е	0.28	0/4629	0.44	0/6275	
2	D	0.36	0/4641	0.45	0/6291	
All	All	0.33	0/18588	0.45	0/25198	

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	4526	0	4542	20	0
1	В	4580	0	4591	30	0
1	Е	4528	0	4544	32	0
2	D	4553	0	4559	25	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
3	D	1	0	0	0	0
3	Е	1	0	0	0	0
4	A	32	0	0	0	0



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	32	0	0	1	0
4	D	32	0	0	0	0
4	Е	32	0	0	0	0
5	A	53	0	30	1	0
5	В	53	0	30	0	0
5	D	53	0	30	1	0
5	Е	53	0	30	2	0
6	A	5	0	4	5	0
6	В	5	0	4	4	0
6	Е	5	0	4	5	0
7	A	31	0	0	1	0
8	В	25	0	17	3	0
8	D	25	0	17	3	0
8	Е	25	0	17	3	0
9	A	260	0	0	2	0
9	В	357	0	0	4	1
9	D	378	0	0	3	0
9	Е	177	0	0	2	1
All	All	19824	0	18419	117	1

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 3.

The worst 5 of 117 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\operatorname{distance}\ (ext{\AA})$	overlap (Å)
6:A:704:F50:HH33	8:D:704:TP9:S1	1.83	1.17
6:A:704:F50:HH31	2:D:582[A]:MET:HG2	1.49	0.93
8:B:704:TP9:S1	6:E:705:F50:HH33	2.11	0.90
2:D:151:ARG:HD3	2:D:182:ILE:HD12	1.57	0.87
6:A:704:F50:CH3	8:D:704:TP9:S1	2.64	0.85

All (1) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
9:B:1097:HOH:O	9:E:806:HOH:O[3_775]	2.19	0.01



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	A	590/677 (87%)	581 (98%)	9 (2%)	0	100	100
1	В	598/677 (88%)	589 (98%)	8 (1%)	1 (0%)	47	55
1	E	590/677 (87%)	577 (98%)	11 (2%)	2 (0%)	41	47
2	D	592/677 (87%)	585 (99%)	7 (1%)	0	100	100
All	All	2370/2708 (88%)	2332 (98%)	35 (2%)	3 (0%)	51	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Е	442	LYS
1	Е	283	GLU
1	В	84	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	487/556~(88%)	483 (99%)	4 (1%)	81 89
1	В	494/556~(89%)	492 (100%)	2 (0%)	91 95
1	E	488/556~(88%)	482 (99%)	6 (1%)	71 82
2	D	488/555 (88%)	482 (99%)	6 (1%)	71 82
All	All	$1957/2223\ (88\%)$	1939 (99%)	18 (1%)	78 87

5 of 18 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
2	D	287	GLN
2	D	619	VAL
2	D	582[B]	MET
1	Е	269	PRO
2	D	265	LYS

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

Mol	Chain	Res	Type
1	A	202	GLN
1	В	202	GLN
1	Ε	202	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	B	ond leng	${ m gths}$	В	ond ang	gles
	IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
Ī	2	SME	D	502	2	7,8,9	1.52	2 (28%)	4,9,11	6.51	3 (75%)

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SME	D	502	2	-	1/6/7/9	-

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
2	D	502	SME	CB-CA	-2.69	1.50	1.53
2	D	502	SME	OE-S	-2.12	1.44	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	D	502	SME	CE-S-CG	10.41	121.39	97.71
2	D	502	SME	OE-S-CE	6.15	118.71	106.25
2	D	502	SME	OE-S-CG	4.85	119.39	106.03

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	502	SME	CB-CG-S-OE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Trino	Chain	ain Res	es Link	В	Bond lengths			Bond angles		
Mol Type Chai	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
4	PXD	D	702	-	30,34,34	3.61	16 (53%)	34,51,51	2.80	13 (38%)	
5	FAD	D	703	-	53,58,58	1.64	10 (18%)	68,89,89	1.30	12 (17%)	
6	F50	Е	705	-	3,4,4	1.66	1 (33%)	3,4,4	2.22	1 (33%)	



Mol	Type	Chain	Res	Link	В	ond leng	$_{ m gths}$	В	ond ang	gles
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	AUJ	A	705	3	25,32,32	2.71	12 (48%)	30,49,49	1.64	7 (23%)
4	PXD	В	702	-	30,34,34	3.33	16 (53%)	34,51,51	2.55	13 (38%)
8	TP9	Е	704	3	21,25,25	2.46	11 (52%)	28,36,36	2.16	10 (35%)
5	FAD	В	703	-	53,58,58	2.37	28 (52%)	68,89,89	1.46	14 (20%)
6	F50	В	705	-	3,4,4	1.72	1 (33%)	3,4,4	3.58	2 (66%)
5	FAD	A	703	-	53,58,58	1.67	11 (20%)	68,89,89	1.33	11 (16%)
8	TP9	D	704	3	21,25,25	2.72	11 (52%)	28,36,36	2.12	10 (35%)
4	PXD	Е	702	-	30,34,34	3.13	16 (53%)	34,51,51	2.47	13 (38%)
4	PXD	A	702	-	30,34,34	3.32	16 (53%)	34,51,51	2.84	14 (41%)
6	F50	A	704	-	3,4,4	1.93	1 (33%)	3,4,4	2.24	1 (33%)
5	FAD	Е	703	-	53,58,58	1.68	11 (20%)	68,89,89	1.32	13 (19%)
8	TP9	В	704	3	21,25,25	2.63	10 (47%)	28,36,36	2.07	11 (39%)

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
4	PXD	D	702	-	-	9/24/26/26	0/3/3/3
5	FAD	D	703	-	-	3/30/50/50	0/6/6/6
6	F50	Е	705	-	-	0/0/2/2	-
7	AUJ	A	705	3	-	5/17/26/26	0/2/2/2
4	PXD	В	702	-	-	7/24/26/26	0/3/3/3
8	TP9	E	704	3	-	5/17/22/22	0/1/1/1
5	FAD	В	703	-	-	3/30/50/50	0/6/6/6
6	F50	В	705	-	-	0/0/2/2	-
5	FAD	A	703	-	-	3/30/50/50	0/6/6/6
8	TP9	D	704	3	-	5/17/22/22	0/1/1/1
4	PXD	E	702	-	-	8/24/26/26	0/3/3/3
4	PXD	A	702	-	-	8/24/26/26	0/3/3/3
6	F50	A	704	-	-	0/0/2/2	-
5	FAD	E	703	-	-	4/30/50/50	0/6/6/6
8	TP9	В	704	3	-	7/17/22/22	0/1/1/1

The worst 5 of 171 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$Ideal(\AA)$
4	D	702	PXD	OAC-SBF	-12.61	1.29	1.43
4	A	702	PXD	OAC-SBF	-9.98	1.32	1.43
4	В	702	PXD	OAC-SBF	-9.40	1.32	1.43
4	Ε	702	PXD	OAC-SBF	-9.12	1.33	1.43
8	D	704	TP9	C4-N3	6.87	1.41	1.32

The worst 5 of 145 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	702	PXD	CBA-SBF-NAR	9.85	117.79	106.68
4	Е	702	PXD	OAD-SBF-OAC	-8.25	109.40	119.55
4	D	702	PXD	OAD-SBF-OAC	-7.91	109.83	119.55
4	D	702	PXD	CBA-SBF-NAR	7.58	115.23	106.68
4	В	702	PXD	CBA-SBF-NAR	7.34	114.96	106.68

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	PXD	OAU-CAN-CBC-FAE
4	A	702	PXD	OAU-CAN-CBC-FAF
4	A	702	PXD	CAW-CBA-SBF-NAR
4	A	702	PXD	CAY-CBA-SBF-NAR
4	В	702	PXD	CAW-CBA-SBF-NAR

There are no ring outliers.

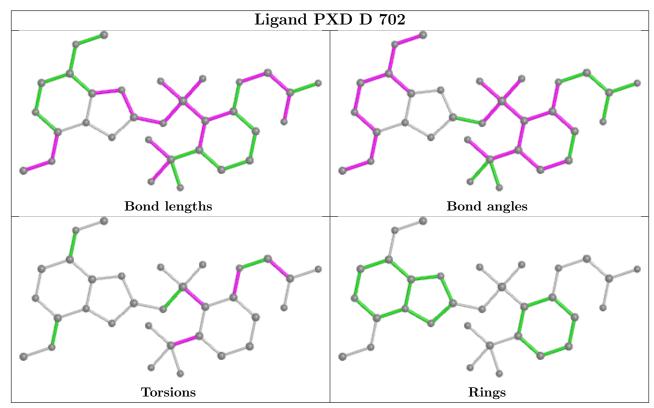
11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	703	FAD	1	0
6	Е	705	F50	5	0
7	A	705	AUJ	1	0
4	В	702	PXD	1	0
8	Ε	704	TP9	3	0
6	В	705	F50	4	0
5	A	703	FAD	1	0
8	D	704	TP9	3	0
6	A	704	F50	5	0
5	Е	703	FAD	2	0
8	В	704	TP9	3	0

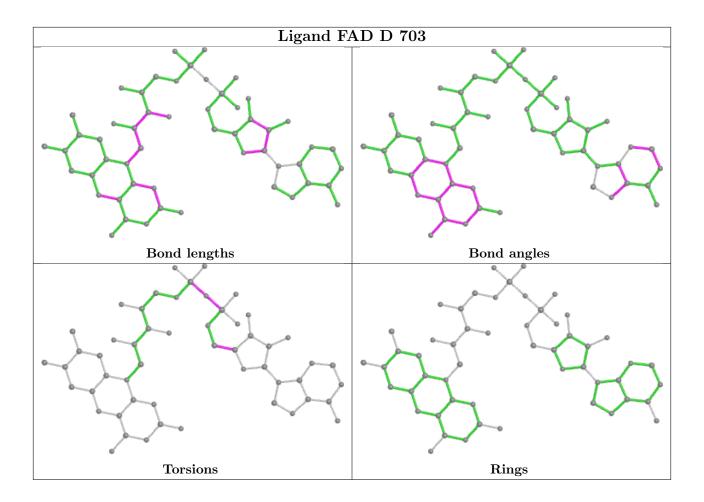
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



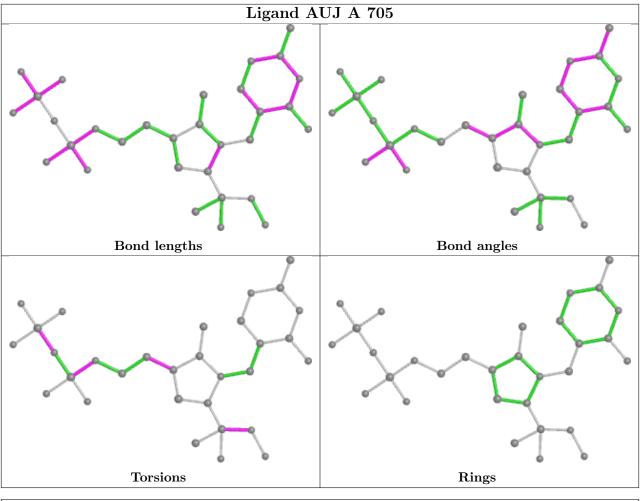
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within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

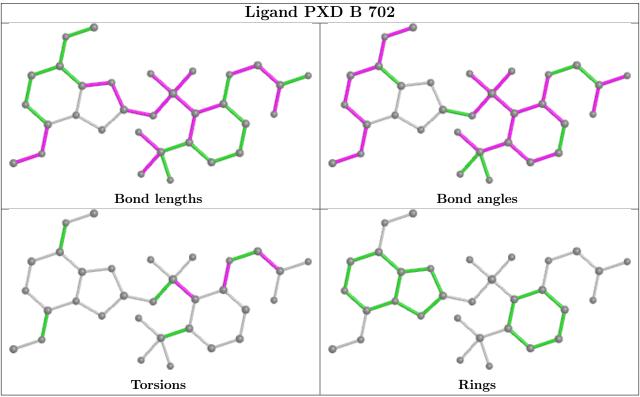




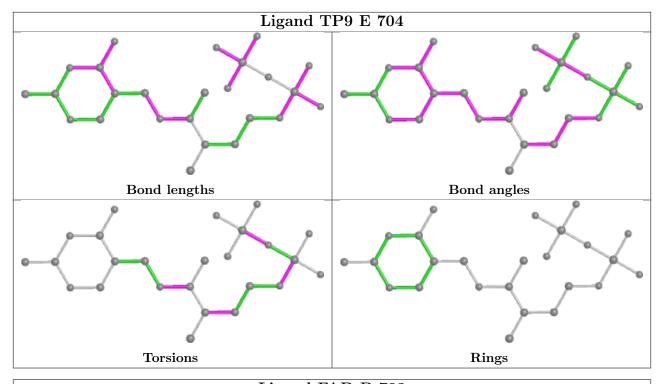


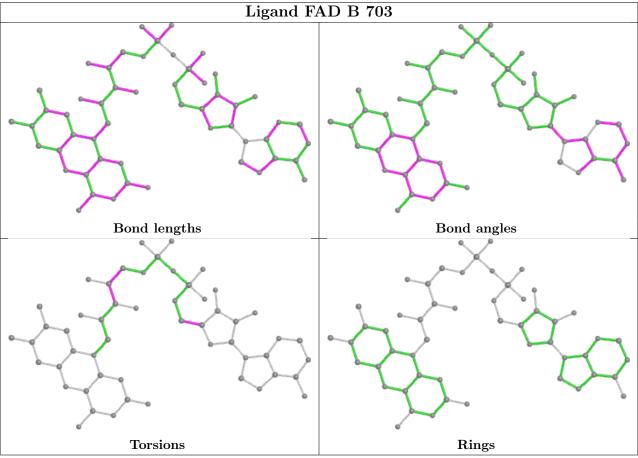




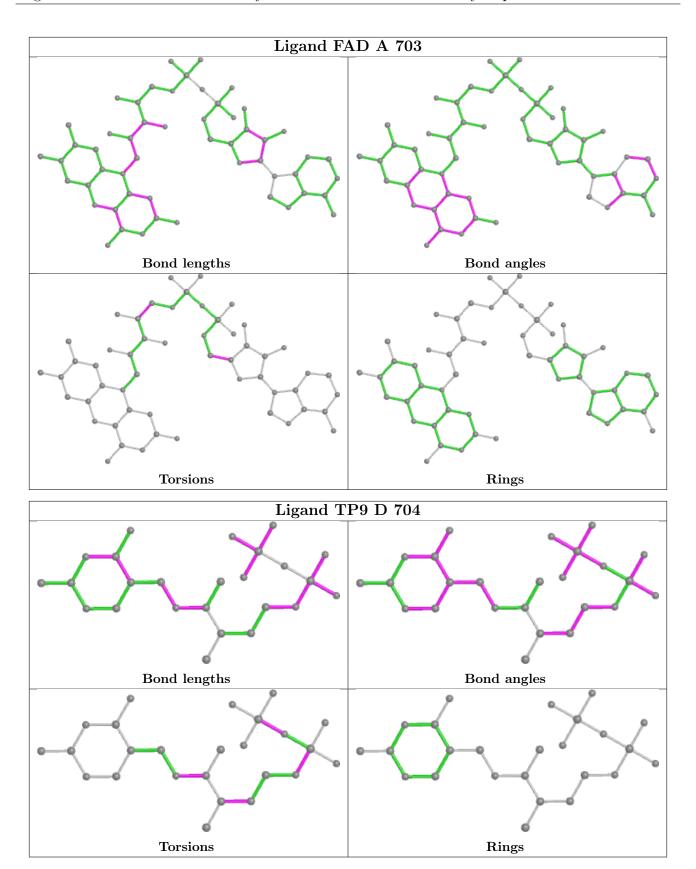




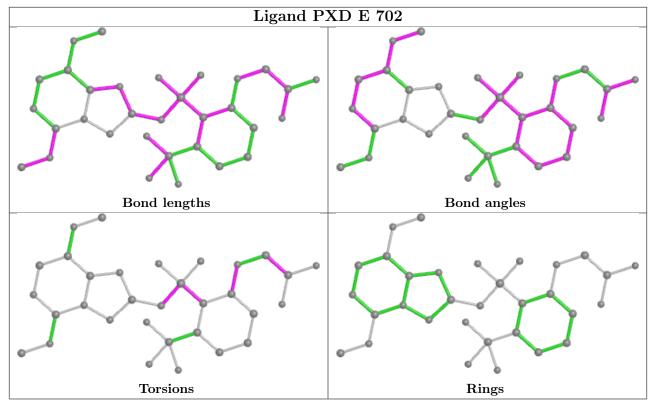


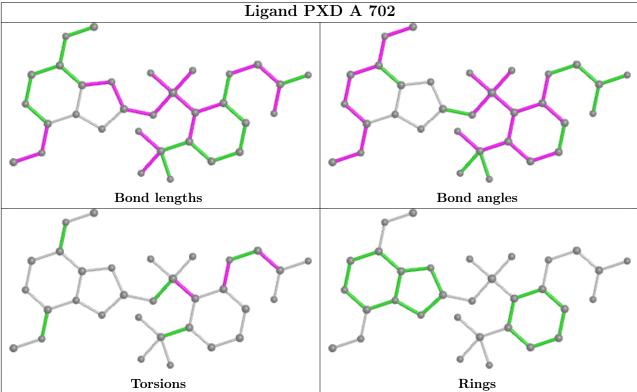




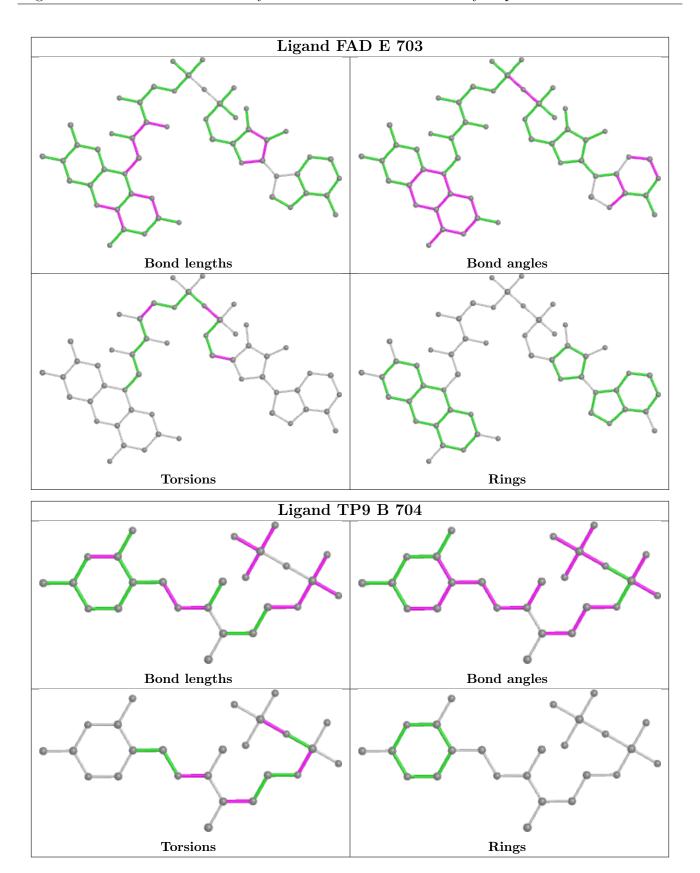














5.7 Other polymers (i)

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<rsrz></rsrz>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	591/677 (87%)	-0.08	24 (4%) 37 48	20, 34, 59, 97	0
1	В	598/677 (88%)	-0.23	9 (1%) 73 81	19, 28, 47, 97	0
1	E	592/677 (87%)	0.33	59 (9%) 7 11	23, 44, 83, 128	0
2	D	595/677 (87%)	-0.22	7 (1%) 79 85	16, 26, 47, 77	0
All	All	2376/2708 (87%)	-0.05	99 (4%) 36 47	16, 32, 66, 128	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	268	LEU	7.3
1	Е	264	THR	6.4
2	D	268	LEU	5.9
1	Е	284	PHE	5.7
1	A	264	THR	5.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	SME	D	502	9/10	0.98	0.12	22,23,38,63	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

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

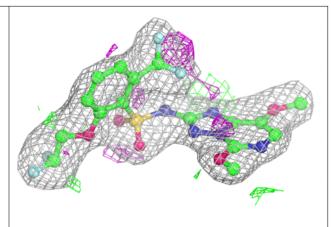
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ m \AA}^2)$	Q<0.9
6	F50	В	705	5/5	0.87	0.35	27,30,35,35	5
6	F50	A	704	5/5	0.89	0.32	22,39,43,43	5
6	F50	E	705	5/5	0.93	0.29	38,39,42,43	5
4	PXD	Ε	702	32/32	0.96	0.10	33,38,60,66	0
5	FAD	Ε	703	53/53	0.96	0.11	32,39,50,50	0
3	MG	Ε	701	1/1	0.96	0.07	26,26,26,26	0
3	MG	D	701	1/1	0.96	0.07	20,20,20,20	0
4	PXD	A	702	32/32	0.96	0.11	23,30,52,58	0
4	PXD	В	702	32/32	0.97	0.11	21,31,48,54	0
3	MG	В	701	1/1	0.97	0.06	23,23,23,23	0
4	PXD	D	702	32/32	0.97	0.11	15,27,45,55	0
5	FAD	A	703	53/53	0.97	0.10	21,29,34,36	0
7	AUJ	A	705	31/31	0.97	0.15	15,24,37,38	3
8	TP9	В	704	25/25	0.97	0.14	17,24,29,40	0
8	TP9	Ε	704	25/25	0.97	0.14	22,26,34,40	0
8	TP9	D	704	25/25	0.97	0.14	14,20,26,39	0
3	MG	A	701	1/1	0.98	0.10	23,23,23,23	0
5	FAD	D	703	53/53	0.98	0.14	13,20,24,33	0
5	FAD	В	703	53/53	0.98	0.11	16,24,27,30	0

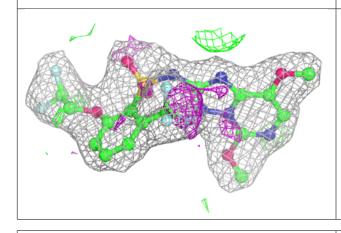
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

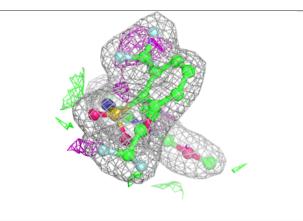


Electron density around PXD E 702:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

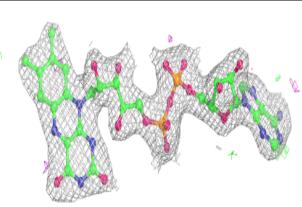


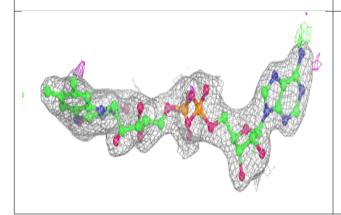


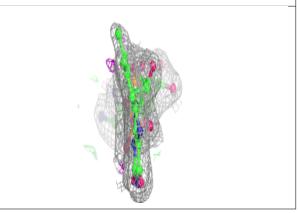


Electron density around FAD E 703:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



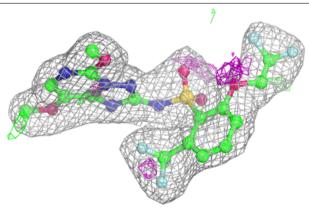


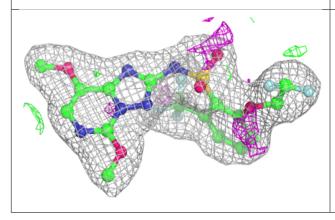


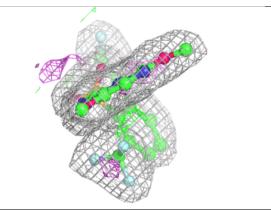


Electron density around PXD A 702:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

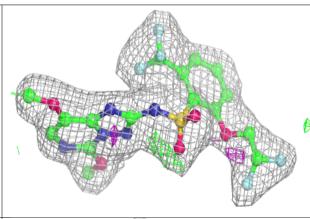


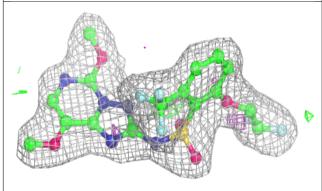


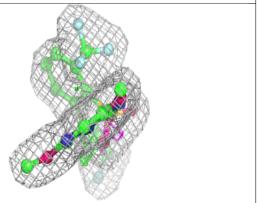


Electron density around PXD B 702:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



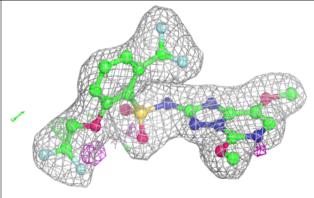


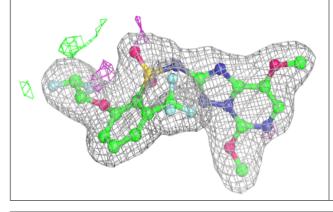


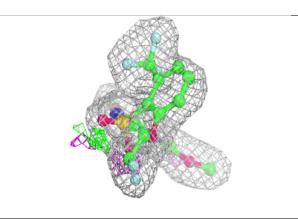


Electron density around PXD D 702:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

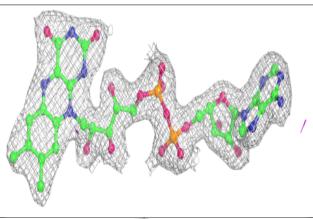


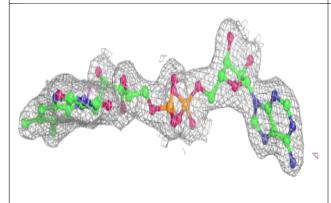


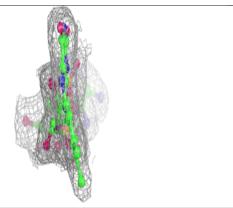


Electron density around FAD A 703:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









Electron density around AUJ A 705: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around TP9 B 704: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

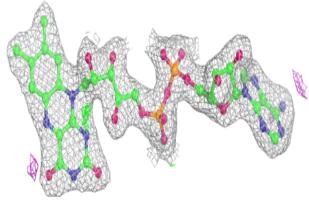


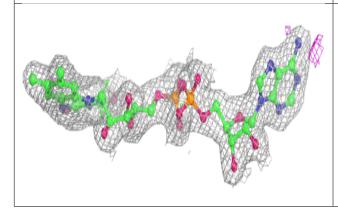
Electron density around TP9 E 704: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around TP9 D 704: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o ext{-}{ m DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

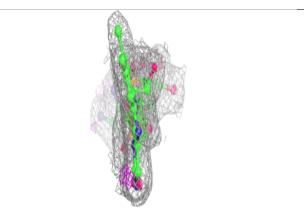


Electron density around FAD D 703:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

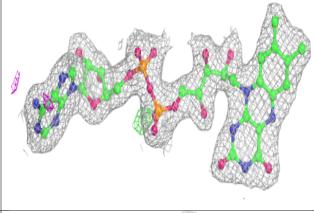


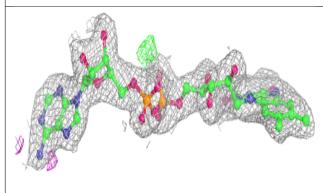


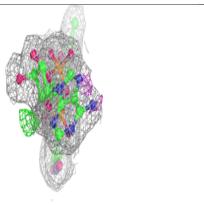


Electron density around FAD B 703:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

