Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 07:37 AM JST

PDB ID	:	7F79
Title	:	Crystal structure of glutamate dehydrogenase 3 from Candida albicans in complex with alpha-ketoglutarate and NADPH
Authors	:	Li, N.; Wang, W.; Zeng, X.; Liu, M.; Li, M.; Li, C.; Wang, M.
Deposited on	:	2021-06-28
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

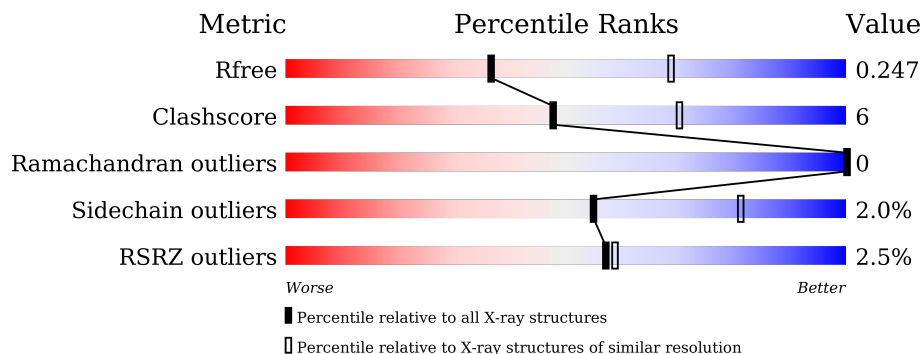|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		2.0%
RSRZ outliers		2.5%

Worse   Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	484	.% 82% 12% 6%
1	B	484	81% 12% 7%
1	C	484	78% 17% 5%
1	D	484	4% 76% 17% 6%
1	E	484	6% 80% 13% 7%
1	F	484	2% 80% 14% 6%

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
3	AKG	A	502	-	-	X	-
3	AKG	C	502	-	X	-	-
3	AKG	D	502	-	-	X	-

2   Entry composition   ⓘ

There are 5 unique types of molecules in this entry. The entry contains 21545 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	1	0
			3495	2214	593	673	15			
1	B	452	Total	C	N	O	S	0	0	0
			3455	2190	588	662	15			
1	C	458	Total	C	N	O	S	0	0	0
			3506	2220	597	674	15			
1	D	454	Total	C	N	O	S	0	0	0
			3475	2201	591	669	14			
1	E	448	Total	C	N	O	S	0	0	0
			3428	2175	582	657	14			
1	F	455	Total	C	N	O	S	0	0	0
			3482	2206	592	670	14			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A1D8PMH8
A	-18	GLY	-	expression tag	UNP A0A1D8PMH8
A	-17	SER	-	expression tag	UNP A0A1D8PMH8
A	-16	SER	-	expression tag	UNP A0A1D8PMH8
A	-15	HIS	-	expression tag	UNP A0A1D8PMH8
A	-14	HIS	-	expression tag	UNP A0A1D8PMH8
A	-13	HIS	-	expression tag	UNP A0A1D8PMH8
A	-12	HIS	-	expression tag	UNP A0A1D8PMH8
A	-11	HIS	-	expression tag	UNP A0A1D8PMH8
A	-10	HIS	-	expression tag	UNP A0A1D8PMH8
A	-9	SER	-	expression tag	UNP A0A1D8PMH8
A	-8	SER	-	expression tag	UNP A0A1D8PMH8
A	-7	GLY	-	expression tag	UNP A0A1D8PMH8
A	-6	LEU	-	expression tag	UNP A0A1D8PMH8
A	-5	VAL	-	expression tag	UNP A0A1D8PMH8
A	-4	PRO	-	expression tag	UNP A0A1D8PMH8
A	-3	ARG	-	expression tag	UNP A0A1D8PMH8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A1D8PMH8
A	-1	SER	-	expression tag	UNP A0A1D8PMH8
A	0	HIS	-	expression tag	UNP A0A1D8PMH8
A	457	LEU	-	expression tag	UNP A0A1D8PMH8
A	458	GLU	-	expression tag	UNP A0A1D8PMH8
A	459	HIS	-	expression tag	UNP A0A1D8PMH8
A	460	HIS	-	expression tag	UNP A0A1D8PMH8
A	461	HIS	-	expression tag	UNP A0A1D8PMH8
A	462	HIS	-	expression tag	UNP A0A1D8PMH8
A	463	HIS	-	expression tag	UNP A0A1D8PMH8
A	464	HIS	-	expression tag	UNP A0A1D8PMH8
B	-19	MET	-	initiating methionine	UNP A0A1D8PMH8
B	-18	GLY	-	expression tag	UNP A0A1D8PMH8
B	-17	SER	-	expression tag	UNP A0A1D8PMH8
B	-16	SER	-	expression tag	UNP A0A1D8PMH8
B	-15	HIS	-	expression tag	UNP A0A1D8PMH8
B	-14	HIS	-	expression tag	UNP A0A1D8PMH8
B	-13	HIS	-	expression tag	UNP A0A1D8PMH8
B	-12	HIS	-	expression tag	UNP A0A1D8PMH8
B	-11	HIS	-	expression tag	UNP A0A1D8PMH8
B	-10	HIS	-	expression tag	UNP A0A1D8PMH8
B	-9	SER	-	expression tag	UNP A0A1D8PMH8
B	-8	SER	-	expression tag	UNP A0A1D8PMH8
B	-7	GLY	-	expression tag	UNP A0A1D8PMH8
B	-6	LEU	-	expression tag	UNP A0A1D8PMH8
B	-5	VAL	-	expression tag	UNP A0A1D8PMH8
B	-4	PRO	-	expression tag	UNP A0A1D8PMH8
B	-3	ARG	-	expression tag	UNP A0A1D8PMH8
B	-2	GLY	-	expression tag	UNP A0A1D8PMH8
B	-1	SER	-	expression tag	UNP A0A1D8PMH8
B	0	HIS	-	expression tag	UNP A0A1D8PMH8
B	457	LEU	-	expression tag	UNP A0A1D8PMH8
B	458	GLU	-	expression tag	UNP A0A1D8PMH8
B	459	HIS	-	expression tag	UNP A0A1D8PMH8
B	460	HIS	-	expression tag	UNP A0A1D8PMH8
B	461	HIS	-	expression tag	UNP A0A1D8PMH8
B	462	HIS	-	expression tag	UNP A0A1D8PMH8
B	463	HIS	-	expression tag	UNP A0A1D8PMH8
B	464	HIS	-	expression tag	UNP A0A1D8PMH8
C	-19	MET	-	initiating methionine	UNP A0A1D8PMH8
C	-18	GLY	-	expression tag	UNP A0A1D8PMH8
C	-17	SER	-	expression tag	UNP A0A1D8PMH8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	expression tag	UNP A0A1D8PMH8
C	-15	HIS	-	expression tag	UNP A0A1D8PMH8
C	-14	HIS	-	expression tag	UNP A0A1D8PMH8
C	-13	HIS	-	expression tag	UNP A0A1D8PMH8
C	-12	HIS	-	expression tag	UNP A0A1D8PMH8
C	-11	HIS	-	expression tag	UNP A0A1D8PMH8
C	-10	HIS	-	expression tag	UNP A0A1D8PMH8
C	-9	SER	-	expression tag	UNP A0A1D8PMH8
C	-8	SER	-	expression tag	UNP A0A1D8PMH8
C	-7	GLY	-	expression tag	UNP A0A1D8PMH8
C	-6	LEU	-	expression tag	UNP A0A1D8PMH8
C	-5	VAL	-	expression tag	UNP A0A1D8PMH8
C	-4	PRO	-	expression tag	UNP A0A1D8PMH8
C	-3	ARG	-	expression tag	UNP A0A1D8PMH8
C	-2	GLY	-	expression tag	UNP A0A1D8PMH8
C	-1	SER	-	expression tag	UNP A0A1D8PMH8
C	0	HIS	-	expression tag	UNP A0A1D8PMH8
C	457	LEU	-	expression tag	UNP A0A1D8PMH8
C	458	GLU	-	expression tag	UNP A0A1D8PMH8
C	459	HIS	-	expression tag	UNP A0A1D8PMH8
C	460	HIS	-	expression tag	UNP A0A1D8PMH8
C	461	HIS	-	expression tag	UNP A0A1D8PMH8
C	462	HIS	-	expression tag	UNP A0A1D8PMH8
C	463	HIS	-	expression tag	UNP A0A1D8PMH8
C	464	HIS	-	expression tag	UNP A0A1D8PMH8
D	-19	MET	-	initiating methionine	UNP A0A1D8PMH8
D	-18	GLY	-	expression tag	UNP A0A1D8PMH8
D	-17	SER	-	expression tag	UNP A0A1D8PMH8
D	-16	SER	-	expression tag	UNP A0A1D8PMH8
D	-15	HIS	-	expression tag	UNP A0A1D8PMH8
D	-14	HIS	-	expression tag	UNP A0A1D8PMH8
D	-13	HIS	-	expression tag	UNP A0A1D8PMH8
D	-12	HIS	-	expression tag	UNP A0A1D8PMH8
D	-11	HIS	-	expression tag	UNP A0A1D8PMH8
D	-10	HIS	-	expression tag	UNP A0A1D8PMH8
D	-9	SER	-	expression tag	UNP A0A1D8PMH8
D	-8	SER	-	expression tag	UNP A0A1D8PMH8
D	-7	GLY	-	expression tag	UNP A0A1D8PMH8
D	-6	LEU	-	expression tag	UNP A0A1D8PMH8
D	-5	VAL	-	expression tag	UNP A0A1D8PMH8
D	-4	PRO	-	expression tag	UNP A0A1D8PMH8
D	-3	ARG	-	expression tag	UNP A0A1D8PMH8

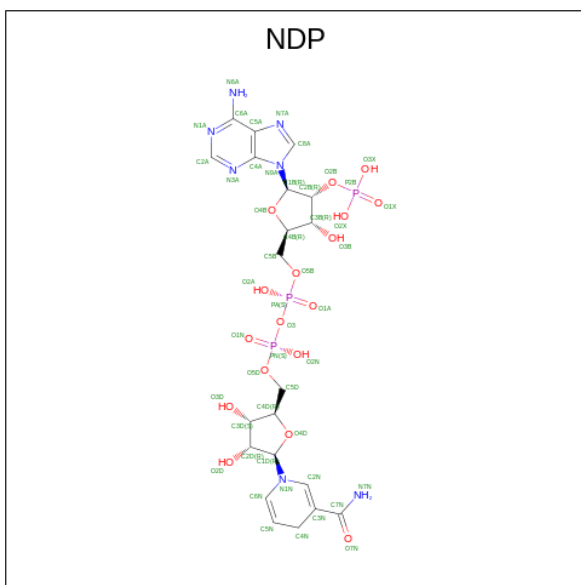*Continued on next page...*

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP A0A1D8PMH8
D	-1	SER	-	expression tag	UNP A0A1D8PMH8
D	0	HIS	-	expression tag	UNP A0A1D8PMH8
D	457	LEU	-	expression tag	UNP A0A1D8PMH8
D	458	GLU	-	expression tag	UNP A0A1D8PMH8
D	459	HIS	-	expression tag	UNP A0A1D8PMH8
D	460	HIS	-	expression tag	UNP A0A1D8PMH8
D	461	HIS	-	expression tag	UNP A0A1D8PMH8
D	462	HIS	-	expression tag	UNP A0A1D8PMH8
D	463	HIS	-	expression tag	UNP A0A1D8PMH8
D	464	HIS	-	expression tag	UNP A0A1D8PMH8
E	-19	MET	-	initiating methionine	UNP A0A1D8PMH8
E	-18	GLY	-	expression tag	UNP A0A1D8PMH8
E	-17	SER	-	expression tag	UNP A0A1D8PMH8
E	-16	SER	-	expression tag	UNP A0A1D8PMH8
E	-15	HIS	-	expression tag	UNP A0A1D8PMH8
E	-14	HIS	-	expression tag	UNP A0A1D8PMH8
E	-13	HIS	-	expression tag	UNP A0A1D8PMH8
E	-12	HIS	-	expression tag	UNP A0A1D8PMH8
E	-11	HIS	-	expression tag	UNP A0A1D8PMH8
E	-10	HIS	-	expression tag	UNP A0A1D8PMH8
E	-9	SER	-	expression tag	UNP A0A1D8PMH8
E	-8	SER	-	expression tag	UNP A0A1D8PMH8
E	-7	GLY	-	expression tag	UNP A0A1D8PMH8
E	-6	LEU	-	expression tag	UNP A0A1D8PMH8
E	-5	VAL	-	expression tag	UNP A0A1D8PMH8
E	-4	PRO	-	expression tag	UNP A0A1D8PMH8
E	-3	ARG	-	expression tag	UNP A0A1D8PMH8
E	-2	GLY	-	expression tag	UNP A0A1D8PMH8
E	-1	SER	-	expression tag	UNP A0A1D8PMH8
E	0	HIS	-	expression tag	UNP A0A1D8PMH8
E	457	LEU	-	expression tag	UNP A0A1D8PMH8
E	458	GLU	-	expression tag	UNP A0A1D8PMH8
E	459	HIS	-	expression tag	UNP A0A1D8PMH8
E	460	HIS	-	expression tag	UNP A0A1D8PMH8
E	461	HIS	-	expression tag	UNP A0A1D8PMH8
E	462	HIS	-	expression tag	UNP A0A1D8PMH8
E	463	HIS	-	expression tag	UNP A0A1D8PMH8
E	464	HIS	-	expression tag	UNP A0A1D8PMH8
F	-19	MET	-	initiating methionine	UNP A0A1D8PMH8
F	-18	GLY	-	expression tag	UNP A0A1D8PMH8
F	-17	SER	-	expression tag	UNP A0A1D8PMH8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-16	SER	-	expression tag	UNP A0A1D8PMH8
F	-15	HIS	-	expression tag	UNP A0A1D8PMH8
F	-14	HIS	-	expression tag	UNP A0A1D8PMH8
F	-13	HIS	-	expression tag	UNP A0A1D8PMH8
F	-12	HIS	-	expression tag	UNP A0A1D8PMH8
F	-11	HIS	-	expression tag	UNP A0A1D8PMH8
F	-10	HIS	-	expression tag	UNP A0A1D8PMH8
F	-9	SER	-	expression tag	UNP A0A1D8PMH8
F	-8	SER	-	expression tag	UNP A0A1D8PMH8
F	-7	GLY	-	expression tag	UNP A0A1D8PMH8
F	-6	LEU	-	expression tag	UNP A0A1D8PMH8
F	-5	VAL	-	expression tag	UNP A0A1D8PMH8
F	-4	PRO	-	expression tag	UNP A0A1D8PMH8
F	-3	ARG	-	expression tag	UNP A0A1D8PMH8
F	-2	GLY	-	expression tag	UNP A0A1D8PMH8
F	-1	SER	-	expression tag	UNP A0A1D8PMH8
F	0	HIS	-	expression tag	UNP A0A1D8PMH8
F	457	LEU	-	expression tag	UNP A0A1D8PMH8
F	458	GLU	-	expression tag	UNP A0A1D8PMH8
F	459	HIS	-	expression tag	UNP A0A1D8PMH8
F	460	HIS	-	expression tag	UNP A0A1D8PMH8
F	461	HIS	-	expression tag	UNP A0A1D8PMH8
F	462	HIS	-	expression tag	UNP A0A1D8PMH8
F	463	HIS	-	expression tag	UNP A0A1D8PMH8
F	464	HIS	-	expression tag	UNP A0A1D8PMH8

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).
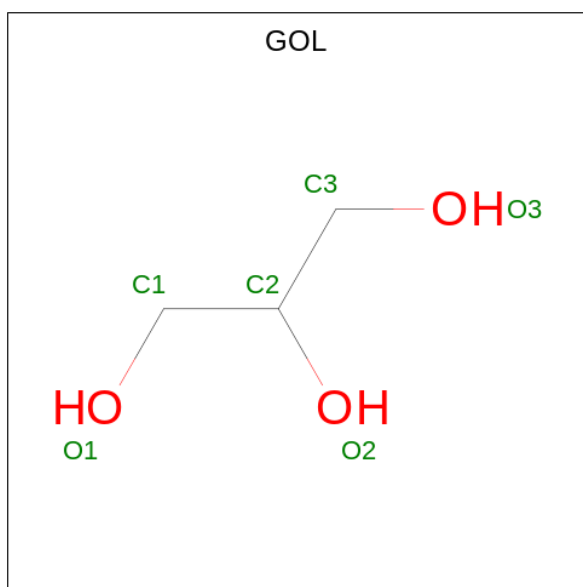
NDP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$) (labeled as "Ligand of Interest" by depositor).
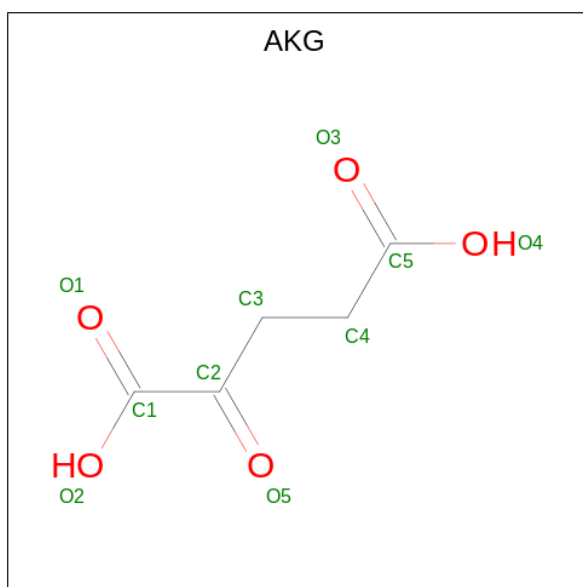
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 10	C 5	O 5	0	0
3	B	1	Total 10	C 5	O 5	0	0
3	C	1	Total 10	C 5	O 5	0	0
3	D	1	Total 10	C 5	O 5	0	0
3	E	1	Total 10	C 5	O 5	0	0
3	F	1	Total 10	C 5	O 5	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1 C2

HO

O1

OH

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total 71	O 71	0	0
5	B	46	Total 46	O 46	0	0
5	C	77	Total 77	O 77	0	0
5	D	34	Total 34	O 34	0	0
5	E	46	Total 46	O 46	0	0
5	F	52	Total 52	O 52	0	0

WORLDWIDE

PDB

PROTEIN DATA BANK

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: Glutamate dehydrogenase
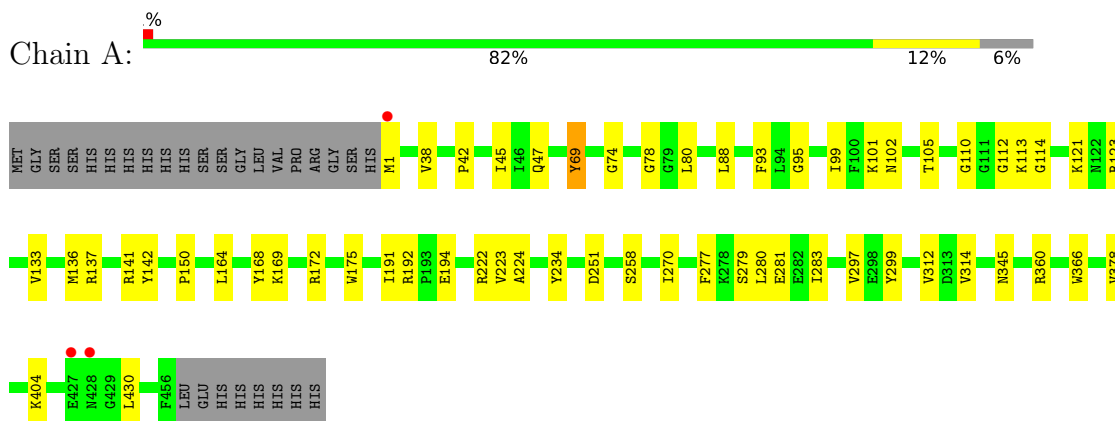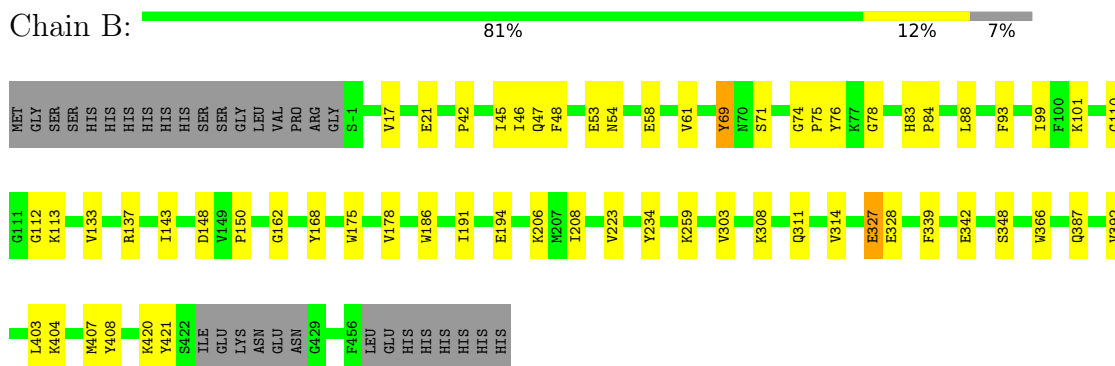
Chain A:
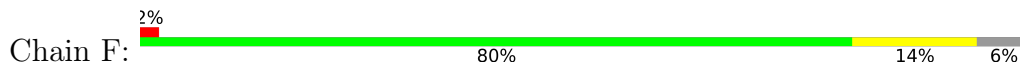
• Molecule 1: Glutamate dehydrogenase

Chain B:

• Molecule 1: Glutamate dehydrogenase

Chain C:

• Molecule 1: Glutamate dehydrogenase

Chain D:
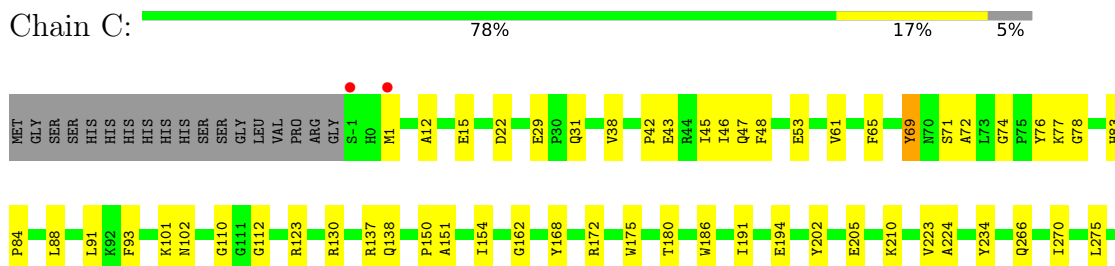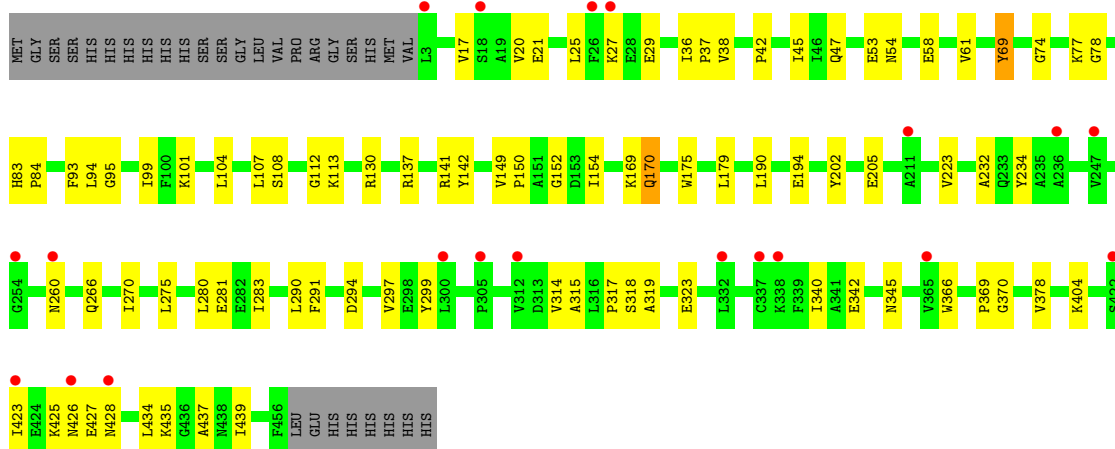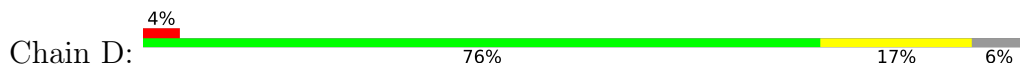
• Molecule 1: Glutamate dehydrogenase

Chain E:

• Molecule 1: Glutamate dehydrogenase

Chain F:
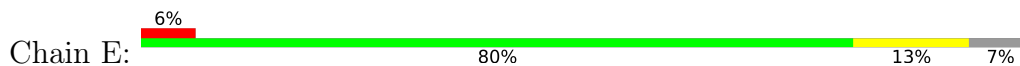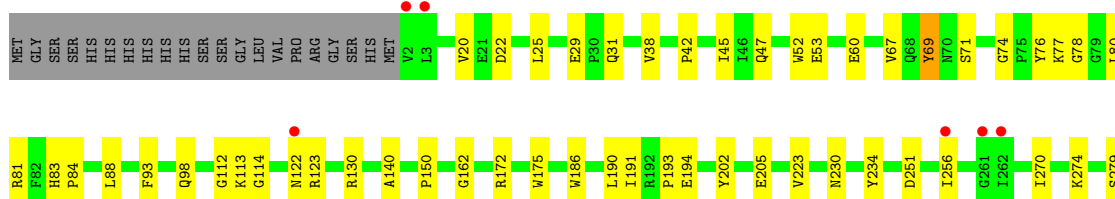
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.28Å 155.22Å 98.81Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	44.80 – 2.70 46.88 – 2.67	Depositor EDS
% Data completeness (in resolution range)	84.0 (44.80-2.70) 82.2 (46.88-2.67)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.199 , 0.247 0.199 , 0.247	Depositor DCC
R_{free} test set	3358 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 28.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21545	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, GOL, AKG

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	0.32	0/3565	0.50	0/4811
1	B	0.32	0/3522	0.49	0/4752
1	C	0.32	0/3574	0.50	0/4823
1	D	0.30	0/3542	0.49	0/4780
1	E	0.31	0/3494	0.49	0/4715
1	F	0.30	0/3549	0.49	0/4790
All	All	0.31	0/21246	0.49	0/28671

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	3495	0	3455	42	0
1	B	3455	0	3414	39	0
1	C	3506	0	3463	46	0
1	D	3475	0	3430	57	0
1	E	3428	0	3389	39	0
1	F	3482	0	3439	44	0
2	A	48	0	26	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	26	1	0
2	C	48	0	26	3	0
2	D	48	0	26	3	0
2	E	48	0	26	4	0
2	F	48	0	26	4	0
3	A	10	0	4	4	0
3	B	10	0	4	2	0
3	C	10	0	4	3	0
3	D	10	0	4	4	0
3	E	10	0	4	1	0
3	F	10	0	4	2	0
4	A	6	0	8	1	0
4	B	6	0	8	1	0
4	D	12	0	16	3	0
4	E	6	0	8	2	0
5	A	71	0	0	2	0
5	B	46	0	0	3	0
5	C	77	0	0	2	0
5	D	34	0	0	2	0
5	E	46	0	0	1	0
5	F	52	0	0	6	0
All	All	21545	0	20810	256	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 (256) 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:113:LYS:NZ	3:B:502:AKG:O5	2.09	0.86
1:D:78:GLY:O	1:D:150:PRO:HA	1.82	0.78
1:D:101:LYS:NZ	3:D:502:AKG:O2	2.16	0.78
2:E:501:NDP:H72N	4:E:503:GOL:H32	1.48	0.78
1:D:108:SER:H	4:D:504:GOL:H31	1.50	0.76
1:F:113:LYS:NZ	3:F:502:AKG:O2	2.24	0.69
1:D:345:ASN:ND2	2:D:501:NDP:O2D	2.25	0.69
1:C:101:LYS:NZ	3:C:502:AKG:O1	2.26	0.69
1:D:223:VAL:HG22	1:D:314:VAL:HB	1.74	0.67
1:E:45:ILE:HB	1:F:47:GLN:HB2	1.76	0.66
1:E:102:ASN:ND2	1:E:110:GLY:O	2.30	0.65
1:B:53:GLU:OE1	5:B:601:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:ALA:O	5:F:601:HOH:O	2.13	0.65
1:A:102:ASN:ND2	1:A:110:GLY:O	2.30	0.65
1:D:137:ARG:HH21	1:D:170:GLN:HG2	1.59	0.64
1:C:47:GLN:HB2	1:D:45:ILE:HB	1.79	0.63
1:C:137:ARG:NH1	5:C:603:HOH:O	2.31	0.63
1:D:190:LEU:N	5:D:601:HOH:O	2.33	0.62
1:E:288:VAL:O	1:E:292:SER:HB2	2.00	0.62
1:F:20:VAL:HG13	1:F:25:LEU:HD23	1.82	0.61
2:F:501:NDP:O1N	2:F:501:NDP:N7N	2.34	0.61
2:C:501:NDP:H41N	3:C:502:AKG:C2	2.31	0.61
1:D:369:PRO:HG3	1:D:434:LEU:HA	1.83	0.60
1:A:258:SER:HB3	1:A:297:VAL:HG12	1.84	0.60
1:D:74:GLY:HA2	1:F:175:TRP:CD2	2.38	0.59
1:A:45:ILE:HD13	1:A:88:LEU:HD11	1.83	0.59
1:D:77:LYS:NZ	3:D:502:AKG:O4	2.27	0.59
1:F:78:GLY:O	1:F:150:PRO:HA	2.03	0.59
1:C:45:ILE:HB	1:D:47:GLN:HB2	1.85	0.59
1:D:20:VAL:HG13	1:D:25:LEU:HD23	1.84	0.59
2:F:501:NDP:H41N	3:F:502:AKG:C2	2.33	0.58
1:A:223:VAL:HG22	1:A:314:VAL:HB	1.85	0.58
1:E:194:GLU:HG3	1:E:234:TYR:CD1	2.39	0.58
1:A:277:PHE:O	5:A:601:HOH:O	2.18	0.57
1:A:78:GLY:O	1:A:150:PRO:HA	2.05	0.56
1:A:137:ARG:HD3	1:D:137:ARG:CZ	2.35	0.56
1:D:25:LEU:HD22	1:D:439:ILE:HG23	1.86	0.56
1:F:303:VAL:HG11	1:F:308:LYS:HE3	1.87	0.56
2:A:501:NDP:H41N	3:A:502:AKG:C2	2.35	0.56
1:F:279:SER:O	1:F:283:ILE:HG23	2.06	0.56
1:A:74:GLY:HA2	1:E:175:TRP:CD2	2.41	0.56
1:B:101:LYS:NZ	3:B:502:AKG:O1	2.39	0.55
1:D:54:ASN:HD21	1:D:58:GLU:HB2	1.71	0.55
1:A:345:ASN:ND2	2:A:501:NDP:O2D	2.39	0.55
1:D:152:GLY:HA3	4:D:503:GOL:H32	1.89	0.55
1:C:224:ALA:HB2	1:C:312:VAL:HG21	1.89	0.54
1:F:274:LYS:NZ	2:F:501:NDP:O2X	2.31	0.54
2:E:501:NDP:N7N	4:E:503:GOL:H32	2.20	0.54
1:E:256:ILE:HB	1:E:297:VAL:HG11	1.90	0.54
1:E:223:VAL:HG22	1:E:314:VAL:HB	1.88	0.54
1:A:45:ILE:HB	1:B:47:GLN:HB2	1.89	0.54
1:A:360:ARG:HD2	1:A:430:LEU:O	2.08	0.54
1:F:80:LEU:HA	1:F:114:GLY:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:THR:HG23	1:E:186:TRP:HD1	1.72	0.53
1:F:360:ARG:HD2	1:F:430:LEU:O	2.08	0.53
1:F:223:VAL:HG22	1:F:314:VAL:HB	1.90	0.53
1:E:83:HIS:CG	1:E:84:PRO:HD2	2.44	0.53
1:A:38:VAL:HG22	1:B:61:VAL:HG21	1.91	0.53
1:B:194:GLU:HG3	1:B:234:TYR:CD1	2.43	0.53
1:F:53:GLU:O	1:F:130:ARG:HD2	2.09	0.53
1:A:121:LYS:NZ	2:A:501:NDP:O3X	2.31	0.52
1:B:133:VAL:O	1:B:137:ARG:HG3	2.09	0.52
2:C:501:NDP:H41N	3:C:502:AKG:C1	2.40	0.52
1:A:168:TYR:CE2	1:A:172:ARG:HG3	2.45	0.52
1:B:54:ASN:HD21	1:B:58:GLU:HB2	1.73	0.52
1:D:291:PHE:HB3	1:D:297:VAL:HG22	1.92	0.52
1:E:61:VAL:HG21	1:F:38:VAL:HG22	1.90	0.52
1:A:113:LYS:NZ	3:A:502:AKG:O5	2.43	0.52
1:E:279:SER:O	1:E:283:ILE:HG23	2.09	0.51
1:B:223:VAL:HG22	1:B:314:VAL:HB	1.92	0.51
1:A:141:ARG:HD2	1:A:142:TYR:CZ	2.46	0.51
1:C:223:VAL:HG22	1:C:314:VAL:HB	1.92	0.51
1:D:107:LEU:HA	4:D:504:GOL:H2	1.93	0.51
1:D:260:ASN:ND2	1:D:294:ASP:O	2.41	0.51
1:F:191:ILE:N	5:F:602:HOH:O	2.19	0.51
1:C:102:ASN:ND2	1:C:110:GLY:O	2.44	0.50
1:E:47:GLN:HB2	1:F:45:ILE:HB	1.93	0.50
1:F:193:PRO:O	1:F:230:ASN:ND2	2.38	0.50
1:F:190:LEU:N	5:F:602:HOH:O	2.45	0.50
1:B:42:PRO:HG3	1:B:69:TYR:CZ	2.46	0.50
1:A:47:GLN:HB2	1:B:45:ILE:HB	1.93	0.50
1:D:104:LEU:HD11	1:D:437:ALA:HB1	1.93	0.50
1:C:78:GLY:O	1:C:150:PRO:HA	2.12	0.50
1:E:78:GLY:O	1:E:150:PRO:HA	2.12	0.50
1:D:17:VAL:O	1:D:21:GLU:HG3	2.13	0.49
1:D:74:GLY:HA2	1:F:175:TRP:CE2	2.47	0.49
1:F:202:TYR:O	1:F:205:GLU:HB2	2.12	0.49
1:E:98:GLN:NE2	1:E:101:LYS:HD2	2.28	0.49
1:F:122:ASN:HB2	5:F:621:HOH:O	2.13	0.49
1:F:194:GLU:HG3	1:F:234:TYR:CD1	2.47	0.49
1:E:256:ILE:HB	1:E:297:VAL:CG1	2.42	0.48
1:B:78:GLY:O	1:B:150:PRO:HA	2.13	0.48
1:E:15:GLU:OE2	1:E:434:LEU:HD21	2.13	0.48
1:E:192:ARG:O	1:E:192:ARG:NH1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:VAL:HG11	1:B:308:LYS:HE3	1.94	0.48
1:C:38:VAL:HG22	1:D:61:VAL:HG21	1.94	0.48
1:D:78:GLY:HA3	1:D:112:GLY:O	2.13	0.48
1:A:280:LEU:O	1:A:283:ILE:HG13	2.14	0.48
1:C:175:TRP:CD2	1:E:74:GLY:HA2	2.48	0.48
1:F:78:GLY:HA3	1:F:112:GLY:O	2.13	0.48
1:A:194:GLU:HG3	1:A:234:TYR:CD1	2.48	0.48
1:E:270:ILE:HG12	1:E:283:ILE:HD13	1.96	0.48
1:B:78:GLY:HA3	1:B:112:GLY:O	2.12	0.48
1:D:95:GLY:O	1:D:99:ILE:HG13	2.14	0.48
1:E:78:GLY:HA3	1:E:112:GLY:O	2.14	0.48
1:C:12:ALA:O	1:C:15:GLU:HG3	2.14	0.48
1:C:303:VAL:HG11	1:C:308:LYS:HE3	1.95	0.47
1:B:54:ASN:ND2	1:B:58:GLU:HB2	2.29	0.47
2:D:501:NDP:H41N	3:D:502:AKG:C2	2.43	0.47
1:A:101:LYS:NZ	3:A:502:AKG:O2	2.40	0.47
1:B:342:GLU:OE2	1:B:348:SER:N	2.45	0.47
1:E:17:VAL:O	1:E:21:GLU:HG3	2.15	0.47
1:A:69:TYR:HB3	1:A:99:ILE:HD11	1.95	0.47
1:A:169:LYS:HZ1	1:C:72:ALA:HA	1.79	0.47
1:A:175:TRP:CD2	1:C:74:GLY:HA2	2.50	0.47
1:D:36:ILE:HG23	1:D:37:PRO:HD3	1.97	0.47
1:E:46:ILE:HG22	1:E:48:PHE:HD2	1.80	0.47
1:B:42:PRO:HG3	1:B:69:TYR:CE2	2.50	0.47
1:D:280:LEU:O	1:D:283:ILE:HG13	2.15	0.47
1:F:29:GLU:HG2	1:F:31:GLN:HE22	1.80	0.47
1:E:202:TYR:O	1:E:205:GLU:HB2	2.15	0.46
1:A:78:GLY:HA3	1:A:112:GLY:O	2.15	0.46
1:B:17:VAL:O	1:B:21:GLU:HG3	2.15	0.46
1:E:42:PRO:HG3	1:E:69:TYR:CZ	2.49	0.46
1:E:68:GLN:HB3	1:E:76:TYR:CD2	2.51	0.46
1:A:279:SER:O	1:A:283:ILE:HG23	2.16	0.46
1:B:403:LEU:O	1:B:407:MET:HG2	2.15	0.46
1:F:42:PRO:HG3	1:F:69:TYR:CZ	2.50	0.46
1:F:280:LEU:O	1:F:283:ILE:HG13	2.16	0.46
1:F:45:ILE:HD13	1:F:88:LEU:HD11	1.98	0.46
1:F:256:ILE:HB	1:F:297:VAL:HG11	1.97	0.46
1:D:77:LYS:HD2	1:D:149:VAL:HB	1.98	0.46
1:A:80:LEU:HA	1:A:114:GLY:O	2.16	0.46
1:B:71:SER:HB3	1:B:76:TYR:CZ	2.51	0.46
1:D:53:GLU:O	1:D:130:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:MET:HG2	1:A:164:LEU:O	2.16	0.45
1:C:78:GLY:HA3	1:C:112:GLY:O	2.17	0.45
1:E:77:LYS:HE3	1:E:381:SER:HB3	1.98	0.45
1:A:133:VAL:O	1:A:137:ARG:HG3	2.16	0.45
1:C:53:GLU:O	1:C:130:ARG:HD2	2.17	0.45
1:D:194:GLU:HG3	1:D:234:TYR:CD1	2.51	0.45
1:C:45:ILE:HD13	1:C:88:LEU:HD11	1.99	0.45
1:D:137:ARG:NH2	1:D:170:GLN:HG2	2.30	0.45
1:D:281:GLU:HB2	1:D:299:TYR:CZ	2.51	0.45
1:F:251:ASP:HB2	2:F:501:NDP:O2X	2.17	0.45
1:F:256:ILE:HB	1:F:297:VAL:CG1	2.47	0.45
2:B:501:NDP:H72N	4:B:503:GOL:H11	1.82	0.45
1:A:42:PRO:HG3	1:A:69:TYR:CZ	2.51	0.45
1:B:46:ILE:HG22	1:B:48:PHE:HD2	1.82	0.45
1:B:71:SER:HB3	1:B:76:TYR:CE1	2.51	0.45
1:D:141:ARG:HD2	1:D:142:TYR:CZ	2.52	0.45
1:E:68:GLN:HB3	1:E:76:TYR:CE2	2.52	0.45
1:E:306:TRP:NE1	1:E:324:VAL:HG22	2.32	0.45
1:E:137:ARG:NH1	5:E:603:HOH:O	2.45	0.45
1:E:162:GLY:HA2	1:E:186:TRP:CH2	2.52	0.45
1:F:71:SER:HB3	1:F:76:TYR:CE1	2.52	0.45
1:A:105:THR:HG21	1:A:378:VAL:HG13	1.99	0.44
1:F:162:GLY:HA2	1:F:186:TRP:CH2	2.52	0.44
1:B:83:HIS:CG	1:B:84:PRO:HD2	2.53	0.44
1:C:61:VAL:HG21	1:D:38:VAL:HG22	1.98	0.44
1:C:151:ALA:HB2	1:C:180:THR:OG1	2.17	0.44
1:F:357:GLU:OE2	5:F:603:HOH:O	2.21	0.44
1:F:52:TRP:CE2	1:F:60:GLU:HB2	2.53	0.44
1:A:281:GLU:HB2	1:A:299:TYR:CZ	2.53	0.44
1:C:342:GLU:OE2	1:C:348:SER:N	2.46	0.44
1:B:137:ARG:HD3	1:E:137:ARG:CZ	2.48	0.44
1:B:175:TRP:CD2	1:F:74:GLY:HA2	2.52	0.44
1:C:307:THR:O	5:C:601:HOH:O	2.21	0.44
1:E:280:LEU:O	1:E:283:ILE:HG13	2.16	0.44
1:C:71:SER:HB3	1:C:76:TYR:CE1	2.53	0.44
1:C:194:GLU:HG3	1:C:234:TYR:CD1	2.53	0.43
1:C:412:GLU:OE1	1:C:416:LYS:HE3	2.18	0.43
1:B:162:GLY:HA2	1:B:186:TRP:CH2	2.53	0.43
1:B:206:LYS:HD3	1:B:408:TYR:CD1	2.53	0.43
1:D:150:PRO:HD2	1:D:179:LEU:HD23	2.00	0.43
1:A:141:ARG:HD3	5:B:641:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:PRO:HG2	1:D:342:GLU:HA	2.01	0.43
1:C:202:TYR:O	1:C:205:GLU:HB2	2.19	0.43
1:A:191:ILE:HG22	1:A:191:ILE:O	2.18	0.43
2:A:501:NDP:H72N	4:A:503:GOL:H2	1.84	0.43
1:C:46:ILE:HG22	1:C:48:PHE:HD2	1.82	0.43
1:D:315:ALA:HB3	1:D:340:ILE:HG12	2.01	0.43
1:F:42:PRO:HG2	1:F:45:ILE:HD11	2.01	0.43
1:B:69:TYR:CD1	1:B:99:ILE:HD11	2.54	0.43
1:C:279:SER:O	1:C:283:ILE:HG13	2.19	0.43
1:D:94:LEU:HB3	1:D:113:LYS:HG2	2.01	0.43
1:E:168:TYR:CE2	1:E:178:VAL:HG21	2.53	0.43
1:C:77:LYS:HE3	1:C:381:SER:HB3	2.01	0.42
1:C:168:TYR:CE2	1:C:172:ARG:HG3	2.53	0.42
1:C:383:LEU:HD22	1:C:394:TRP:HZ3	1.84	0.42
1:F:45:ILE:HG23	1:F:67:VAL:HG22	2.01	0.42
1:B:387:GLN:HB3	1:B:392:VAL:O	2.19	0.42
1:B:191:ILE:O	1:B:191:ILE:HG22	2.19	0.42
1:C:337:CYS:O	1:C:365:VAL:HG22	2.20	0.42
1:D:42:PRO:HG3	1:D:69:TYR:CZ	2.54	0.42
1:C:191:ILE:HG22	1:C:191:ILE:O	2.19	0.42
1:D:378:VAL:HB	3:D:502:AKG:H32	2.00	0.42
1:B:327:GLU:HG3	1:B:328:GLU:N	2.34	0.42
1:B:75:PRO:O	1:B:110:GLY:N	2.51	0.42
1:C:266:GLN:O	1:C:270:ILE:HG13	2.19	0.42
1:D:17:VAL:HG22	1:D:36:ILE:HD11	2.01	0.42
1:D:319:ALA:HB3	1:D:323:GLU:OE1	2.20	0.42
1:E:104:LEU:HD11	1:E:437:ALA:HB1	2.01	0.42
1:B:168:TYR:CE2	1:B:178:VAL:HG21	2.55	0.42
1:E:54:ASN:HD21	1:E:58:GLU:HB2	1.85	0.42
1:A:169:LYS:NZ	1:C:72:ALA:HA	2.35	0.42
1:D:36:ILE:CG2	1:D:37:PRO:HD3	2.50	0.42
1:F:191:ILE:HG22	1:F:191:ILE:O	2.20	0.42
1:B:74:GLY:HA2	1:D:175:TRP:CD2	2.54	0.42
1:C:162:GLY:HA2	1:C:186:TRP:CH2	2.54	0.42
1:E:344:SER:HA	2:E:501:NDP:H1D	2.00	0.41
1:C:154:ILE:HD11	2:C:501:NDP:H3D	2.01	0.41
1:C:43:GLU:OE1	1:C:76:TYR:OH	2.32	0.41
1:D:426:ASN:C	1:D:428:ASN:H	2.23	0.41
1:E:136:MET:HG2	1:E:164:LEU:O	2.20	0.41
1:F:77:LYS:O	1:F:98:GLN:HG2	2.19	0.41
1:E:91:LEU:HD23	1:E:91:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:NE	5:A:603:HOH:O	2.36	0.41
1:D:266:GLN:O	1:D:270:ILE:HG13	2.21	0.41
1:D:154:ILE:HG12	2:D:501:NDP:H52N	2.02	0.41
1:A:192:ARG:HA	1:A:192:ARG:HD2	1.88	0.41
1:C:319:ALA:HB3	1:C:323:GLU:OE1	2.21	0.41
1:D:83:HIS:CG	1:D:84:PRO:HD2	2.55	0.41
1:D:202:TYR:O	1:D:205:GLU:HB2	2.21	0.41
1:D:266:GLN:HG2	1:D:290:LEU:HG	2.03	0.41
1:C:42:PRO:HG3	1:C:69:TYR:CZ	2.56	0.41
1:C:65:PHE:HB2	1:C:91:LEU:CD1	2.51	0.41
1:C:304:ARG:NH1	1:C:328:GLU:OE1	2.53	0.41
1:A:224:ALA:HB2	1:A:312:VAL:HG21	2.03	0.41
1:A:251:ASP:HB2	2:A:501:NDP:O2X	2.20	0.41
1:B:143:ILE:HG22	1:B:148:ASP:HB3	2.02	0.41
1:C:83:HIS:CG	1:C:84:PRO:HD2	2.56	0.41
1:C:275:LEU:HD23	1:C:275:LEU:HA	1.95	0.41
1:C:360:ARG:HD2	1:C:430:LEU:O	2.20	0.41
1:D:435:LYS:HE3	5:D:620:HOH:O	2.21	0.41
1:F:83:HIS:CG	1:F:84:PRO:HD2	2.56	0.41
1:A:95:GLY:O	1:A:99:ILE:HG13	2.21	0.41
1:A:270:ILE:HG12	1:A:283:ILE:HD13	2.03	0.41
1:C:210:LYS:HG2	1:C:415:TYR:CE2	2.55	0.41
1:F:337:CYS:O	1:F:365:VAL:HG22	2.21	0.41
1:D:342:GLU:OE1	1:D:370:GLY:N	2.51	0.40
1:E:191:ILE:HG22	1:E:191:ILE:O	2.21	0.40
1:A:175:TRP:CE2	1:C:74:GLY:HA2	2.56	0.40
1:D:232:ALA:HB2	1:D:318:SER:HB2	2.02	0.40
1:D:275:LEU:HD23	1:D:275:LEU:HA	1.87	0.40
1:B:45:ILE:HD13	1:B:88:LEU:HD11	2.03	0.40
1:B:88:LEU:HB3	5:B:639:HOH:O	2.22	0.40
1:B:208:ILE:HG12	1:B:339:PHE:CE2	2.56	0.40
1:D:169:LYS:HB3	1:D:169:LYS:HE3	1.93	0.40
1:F:270:ILE:HG12	1:F:283:ILE:HD13	2.02	0.40
1:A:378:VAL:HB	3:A:502:AKG:H41	2.02	0.40
1:B:420:LYS:HD3	1:B:421:TYR:CE2	2.57	0.40
1:D:27:LYS:HE3	1:D:423:ILE:HD13	2.03	0.40
2:E:501:NDP:H41N	3:E:502:AKG:C1	2.51	0.40
1:F:81:ARG:NH1	5:F:608:HOH:O	2.41	0.40
1:F:140:ALA:O	1:F:172:ARG:NH1	2.54	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	455/484 (94%)	443 (97%)	12 (3%)	0	100	100
1	B	448/484 (93%)	434 (97%)	14 (3%)	0	100	100
1	C	456/484 (94%)	441 (97%)	15 (3%)	0	100	100
1	D	452/484 (93%)	437 (97%)	15 (3%)	0	100	100
1	E	444/484 (92%)	429 (97%)	15 (3%)	0	100	100
1	F	453/484 (94%)	440 (97%)	13 (3%)	0	100	100
All	All	2708/2904 (93%)	2624 (97%)	84 (3%)	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	367/391 (94%)	361 (98%)	6 (2%)	62	85
1	B	362/391 (93%)	355 (98%)	7 (2%)	57	82
1	C	368/391 (94%)	358 (97%)	10 (3%)	44	74
1	D	364/391 (93%)	356 (98%)	8 (2%)	52	79
1	E	359/391 (92%)	353 (98%)	6 (2%)	60	84
1	F	365/391 (93%)	358 (98%)	7 (2%)	57	82
All	All	2185/2346 (93%)	2141 (98%)	44 (2%)	55	81

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	69	TYR
1	A	93	PHE
1	A	123	ARG
1	A	366	TRP
1	A	404	LYS
1	B	69	TYR
1	B	93	PHE
1	B	259	LYS
1	B	311	GLN
1	B	327	GLU
1	B	366	TRP
1	B	404	LYS
1	C	1	MET
1	C	22	ASP
1	C	29	GLU
1	C	31	GLN
1	C	69	TYR
1	C	93	PHE
1	C	123	ARG
1	C	138	GLN
1	C	366	TRP
1	C	425	LYS
1	D	29	GLU
1	D	69	TYR
1	D	93	PHE
1	D	170	GLN
1	D	366	TRP
1	D	404	LYS
1	D	425	LYS
1	D	427	GLU
1	E	27	LYS
1	E	29	GLU
1	E	69	TYR
1	E	93	PHE
1	E	123	ARG
1	E	366	TRP
1	F	22	ASP
1	F	69	TYR
1	F	93	PHE
1	F	123	ARG
1	F	366	TRP

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Mol	Chain	Res	Type
1	F	424	GLU
1	F	425	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	31	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	NDP	E	501	-	45,52,52	0.69	0	53,80,80	0.92	4 (7%)
2	NDP	F	501	-	45,52,52	0.70	0	53,80,80	0.97	3 (5%)
4	GOL	B	503	-	5,5,5	1.00	0	5,5,5	0.92	0
2	NDP	C	501	-	45,52,52	0.69	0	53,80,80	0.92	2 (3%)
4	GOL	A	503	-	5,5,5	1.08	0	5,5,5	0.92	0

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Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	GOL	D	503	-	5,5,5	0.94	0	5,5,5	0.91	0
3	AKG	D	502	-	9,9,9	1.05	0	11,11,11	1.83	3 (27%)
3	AKG	F	502	-	9,9,9	1.06	0	11,11,11	1.45	2 (18%)
4	GOL	E	503	-	5,5,5	0.91	0	5,5,5	0.96	0
2	NDP	B	501	-	45,52,52	0.72	0	53,80,80	1.02	3 (5%)
2	NDP	A	501	-	45,52,52	0.70	0	53,80,80	0.96	2 (3%)
3	AKG	B	502	-	9,9,9	1.02	0	11,11,11	1.85	4 (36%)
3	AKG	E	502	-	9,9,9	1.06	0	11,11,11	1.17	0
4	GOL	D	504	-	5,5,5	1.08	0	5,5,5	0.77	0
3	AKG	C	502	-	9,9,9	1.03	0	11,11,11	1.79	3 (27%)
2	NDP	D	501	-	45,52,52	0.68	0	53,80,80	1.03	4 (7%)
3	AKG	A	502	-	9,9,9	0.99	0	11,11,11	2.21	6 (54%)

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	NDP	E	501	-	-	6/30/77/77	0/5/5/5
2	NDP	F	501	-	-	9/30/77/77	0/5/5/5
4	GOL	B	503	-	-	4/4/4/4	-
2	NDP	C	501	-	-	9/30/77/77	0/5/5/5
4	GOL	A	503	-	-	2/4/4/4	-
4	GOL	D	503	-	-	4/4/4/4	-
3	AKG	D	502	-	-	1/9/9/9	-
3	AKG	F	502	-	-	2/9/9/9	-
4	GOL	E	503	-	-	2/4/4/4	-
2	NDP	B	501	-	-	13/30/77/77	0/5/5/5
2	NDP	A	501	-	-	7/30/77/77	0/5/5/5
3	AKG	B	502	-	-	5/9/9/9	-
3	AKG	E	502	-	-	6/9/9/9	-
4	GOL	D	504	-	-	4/4/4/4	-
3	AKG	C	502	-	-	9/9/9/9	-
2	NDP	D	501	-	-	10/30/77/77	0/5/5/5
3	AKG	A	502	-	-	1/9/9/9	-

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NDP	C1B-N9A-C4A	4.35	134.28	126.64
2	F	501	NDP	C1B-N9A-C4A	4.27	134.14	126.64
2	A	501	NDP	C1B-N9A-C4A	4.09	133.82	126.64
3	A	502	AKG	C3-C4-C5	-3.71	105.63	113.60
3	B	502	AKG	C3-C4-C5	-3.56	105.95	113.60
2	D	501	NDP	C1B-N9A-C4A	3.53	132.84	126.64
2	E	501	NDP	C1B-N9A-C4A	3.48	132.76	126.64
3	A	502	AKG	C3-C2-C1	3.19	121.89	115.97
3	D	502	AKG	C3-C4-C5	-3.05	107.03	113.60
2	C	501	NDP	C1B-N9A-C4A	3.03	131.96	126.64
3	A	502	AKG	C4-C3-C2	-2.98	107.41	113.03
3	C	502	AKG	O2-C1-C2	2.86	121.80	113.97
3	C	502	AKG	C3-C2-C1	2.71	121.01	115.97
3	B	502	AKG	O1-C1-C2	-2.54	118.32	121.72
2	A	501	NDP	N3A-C2A-N1A	-2.51	124.75	128.68
3	C	502	AKG	O1-C1-C2	-2.49	118.40	121.72
2	C	501	NDP	N3A-C2A-N1A	-2.48	124.80	128.68
2	B	501	NDP	N3A-C2A-N1A	-2.41	124.92	128.68
2	D	501	NDP	N3A-C2A-N1A	-2.39	124.94	128.68
2	E	501	NDP	N3A-C2A-N1A	-2.34	125.03	128.68
3	D	502	AKG	O4-C5-C4	2.32	121.49	114.03
3	D	502	AKG	C3-C2-C1	2.31	120.26	115.97
3	A	502	AKG	O2-C1-C2	2.29	120.23	113.97
3	B	502	AKG	O2-C1-C2	2.28	120.21	113.97
2	E	501	NDP	C3N-C2N-N1N	-2.28	119.84	123.10
2	D	501	NDP	C4A-C5A-N7A	-2.27	107.03	109.40
3	F	502	AKG	O2-C1-C2	2.26	120.16	113.97
2	E	501	NDP	C4A-C5A-N7A	-2.24	107.07	109.40
2	F	501	NDP	N3A-C2A-N1A	-2.23	125.19	128.68
3	A	502	AKG	O5-C2-C3	-2.17	116.39	121.20
3	F	502	AKG	C3-C4-C5	-2.16	108.96	113.60
3	B	502	AKG	O4-C5-C4	2.15	120.93	114.03
2	F	501	NDP	C4A-C5A-N7A	-2.14	107.17	109.40
2	D	501	NDP	C3N-C2N-N1N	-2.08	120.13	123.10
2	B	501	NDP	C3N-C2N-N1N	-2.02	120.21	123.10
3	A	502	AKG	O1-C1-C2	-2.02	119.03	121.72

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NDP	C5B-O5B-PA-O3
2	B	501	NDP	C5B-O5B-PA-O3
2	B	501	NDP	C5D-O5D-PN-O3
2	B	501	NDP	O4D-C4D-C5D-O5D
2	C	501	NDP	C5B-O5B-PA-O3
2	D	501	NDP	C5B-O5B-PA-O3
2	D	501	NDP	C2B-O2B-P2B-O1X
2	D	501	NDP	O4D-C4D-C5D-O5D
2	E	501	NDP	C5B-O5B-PA-O3
2	F	501	NDP	C5B-O5B-PA-O3
3	B	502	AKG	C1-C2-C3-C4
3	C	502	AKG	O1-C1-C2-O5
3	C	502	AKG	O1-C1-C2-C3
3	C	502	AKG	O2-C1-C2-O5
3	C	502	AKG	O2-C1-C2-C3
3	C	502	AKG	C1-C2-C3-C4
3	C	502	AKG	C2-C3-C4-C5
3	E	502	AKG	O1-C1-C2-C3
3	E	502	AKG	O2-C1-C2-C3
3	F	502	AKG	O2-C1-C2-C3
4	D	503	GOL	O1-C1-C2-C3
4	D	504	GOL	O1-C1-C2-O2
4	D	504	GOL	C1-C2-C3-O3
4	E	503	GOL	O1-C1-C2-O2
4	E	503	GOL	O1-C1-C2-C3
2	B	501	NDP	C3D-C4D-C5D-O5D
2	F	501	NDP	O4D-C4D-C5D-O5D
2	F	501	NDP	C3D-C4D-C5D-O5D
2	D	501	NDP	C3D-C4D-C5D-O5D
3	C	502	AKG	O5-C2-C3-C4
2	C	501	NDP	C3B-C2B-O2B-P2B
3	D	502	AKG	C2-C3-C4-C5
3	E	502	AKG	C2-C3-C4-C5
4	A	503	GOL	O1-C1-C2-C3
4	B	503	GOL	O1-C1-C2-C3
4	B	503	GOL	C1-C2-C3-O3
4	D	503	GOL	C1-C2-C3-O3
4	D	504	GOL	O1-C1-C2-C3
4	B	503	GOL	O1-C1-C2-O2
4	D	503	GOL	O1-C1-C2-O2
4	D	504	GOL	O2-C2-C3-O3
2	A	501	NDP	O4D-C4D-C5D-O5D
2	E	501	NDP	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
4	A	503	GOL	O1-C1-C2-O2
4	B	503	GOL	O2-C2-C3-O3
3	A	502	AKG	C2-C3-C4-C5
3	F	502	AKG	C2-C3-C4-C5
2	E	501	NDP	O4D-C1D-N1N-C6N
2	D	501	NDP	O4B-C4B-C5B-O5B
2	C	501	NDP	C1B-C2B-O2B-P2B
2	D	501	NDP	C2B-O2B-P2B-O2X
2	D	501	NDP	C5D-O5D-PN-O3
2	E	501	NDP	O4B-C4B-C5B-O5B
2	A	501	NDP	O4D-C1D-N1N-C6N
2	D	501	NDP	O4D-C1D-N1N-C6N
2	A	501	NDP	C5B-O5B-PA-O2A
2	B	501	NDP	C5B-O5B-PA-O2A
2	B	501	NDP	C5D-O5D-PN-O2N
2	C	501	NDP	C5B-O5B-PA-O2A
2	D	501	NDP	C5B-O5B-PA-O1A
2	D	501	NDP	C5B-O5B-PA-O2A
2	E	501	NDP	C5B-O5B-PA-O2A
2	F	501	NDP	C5B-O5B-PA-O1A
2	F	501	NDP	C5B-O5B-PA-O2A
3	E	502	AKG	O1-C1-C2-O5
2	F	501	NDP	O4D-C1D-N1N-C6N
2	B	501	NDP	O4D-C1D-N1N-C6N
2	C	501	NDP	O4D-C1D-N1N-C6N
3	E	502	AKG	C3-C4-C5-O3
2	C	501	NDP	C2D-C1D-N1N-C6N
3	B	502	AKG	C2-C3-C4-C5
2	F	501	NDP	O4B-C4B-C5B-O5B
3	E	502	AKG	C3-C4-C5-O4
3	B	502	AKG	O5-C2-C3-C4
2	E	501	NDP	C3D-C4D-C5D-O5D
3	B	502	AKG	C3-C4-C5-O4
2	A	501	NDP	O4B-C4B-C5B-O5B
2	A	501	NDP	C3D-C4D-C5D-O5D
2	F	501	NDP	C2B-O2B-P2B-O1X
2	B	501	NDP	C2D-C1D-N1N-C6N
3	C	502	AKG	C3-C4-C5-O4
3	C	502	AKG	C3-C4-C5-O3
3	B	502	AKG	C3-C4-C5-O3
4	D	503	GOL	O2-C2-C3-O3
2	B	501	NDP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	B	501	NDP	PN-O3-PA-O2A
2	C	501	NDP	PN-O3-PA-O2A
2	A	501	NDP	C5B-O5B-PA-O1A
2	B	501	NDP	C5B-O5B-PA-O1A
2	B	501	NDP	C5D-O5D-PN-O1N
2	C	501	NDP	C5B-O5B-PA-O1A
2	C	501	NDP	O4B-C4B-C5B-O5B
2	B	501	NDP	C3B-C2B-O2B-P2B
2	F	501	NDP	C3B-C2B-O2B-P2B

There are no ring outliers.

17 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	NDP	4	0
2	F	501	NDP	4	0
4	B	503	GOL	1	0
2	C	501	NDP	3	0
4	A	503	GOL	1	0
4	D	503	GOL	1	0
3	D	502	AKG	4	0
3	F	502	AKG	2	0
4	E	503	GOL	2	0
2	B	501	NDP	1	0
2	A	501	NDP	5	0
3	B	502	AKG	2	0
3	E	502	AKG	1	0
4	D	504	GOL	2	0
3	C	502	AKG	3	0
2	D	501	NDP	3	0
3	A	502	AKG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
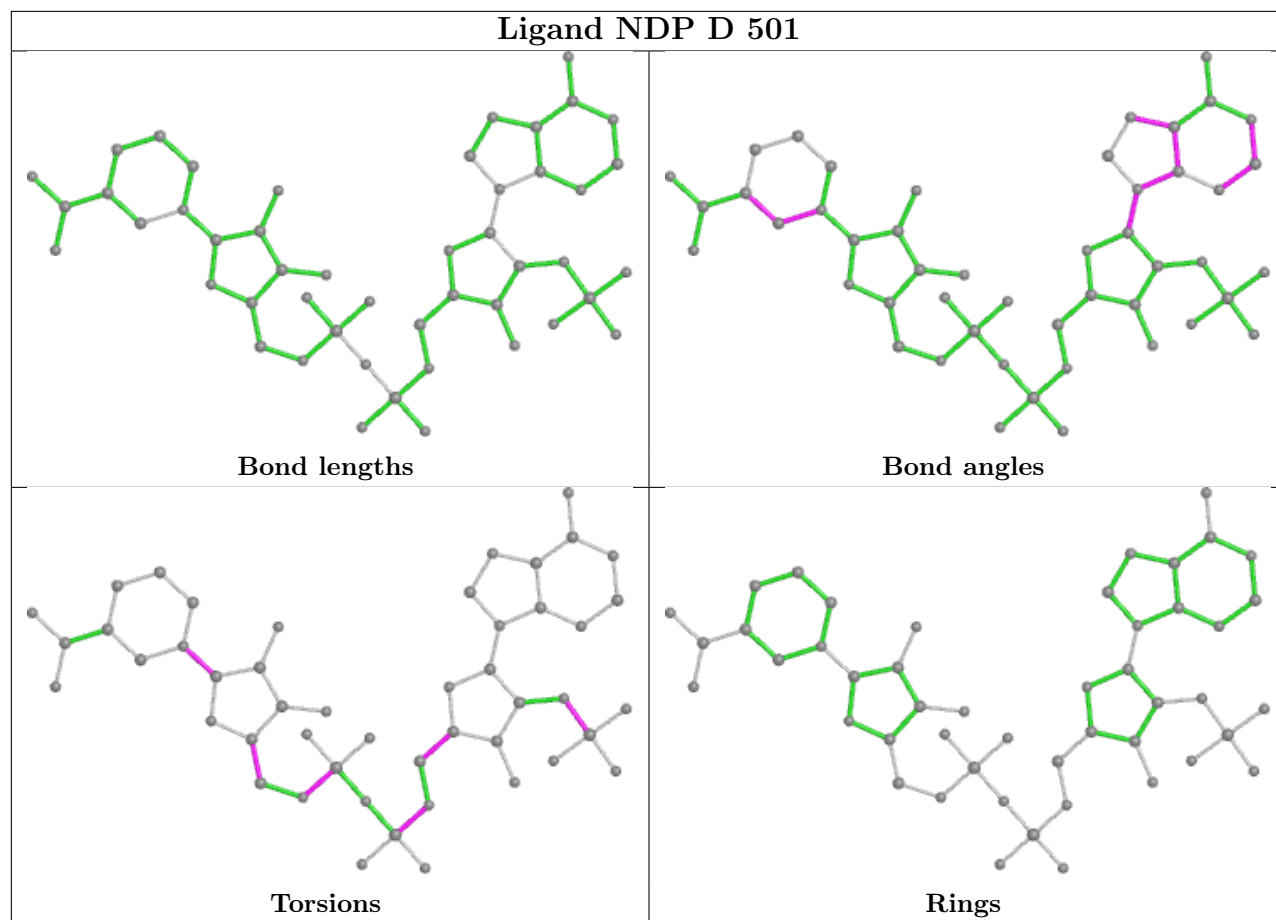
Ligand NDP E 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP F 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand AKG D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand AKG F 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand AKG B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand AKG E 502

Bond lengths

Bond angles

Torsions

Rings

Ligand AKG C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand AKG A 502

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	456/484 (94%)	-0.27	3 (0%) 87	89	19, 34, 56, 100	0
1	B	452/484 (93%)	-0.12	0 100	100	20, 41, 62, 76	0
1	C	458/484 (94%)	-0.36	2 (0%) 92	93	21, 31, 50, 94	0
1	D	454/484 (93%)	0.12	20 (4%) 34	33	26, 49, 78, 97	0
1	E	448/484 (92%)	0.27	31 (6%) 16	15	19, 45, 79, 95	0
1	F	455/484 (94%)	0.07	11 (2%) 59	60	22, 41, 72, 97	0
All	All	2723/2904 (93%)	-0.05	67 (2%) 57	59	19, 39, 73, 100	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	288	VAL	5.2
1	E	259	LYS	4.8
1	E	3	LEU	4.2
1	A	428	ASN	4.2
1	E	291	PHE	4.2
1	E	315	ALA	3.8
1	D	365	VAL	3.7
1	E	314	VAL	3.5
1	E	339	PHE	3.4
1	D	422	SER	3.3
1	F	283	ILE	3.2
1	D	3	LEU	3.2
1	D	423	ILE	3.1
1	F	2	VAL	3.1
1	E	33	LYS	2.9
1	E	361	ASP	2.9
1	E	341	ALA	2.9
1	E	27	LYS	2.8
1	D	26	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	340	ILE	2.8
1	D	312	VAL	2.8
1	E	283	ILE	2.8
1	E	430	LEU	2.7
1	E	415	TYR	2.7
1	E	218	PHE	2.7
1	F	427	GLU	2.7
1	F	262	ILE	2.7
1	E	261	GLY	2.6
1	D	332	LEU	2.6
1	E	266	GLN	2.6
1	D	337	CYS	2.5
1	E	224	ALA	2.5
1	E	289	GLN	2.5
1	F	429	GLY	2.5
1	D	338	LYS	2.4
1	D	27	LYS	2.4
1	D	236	ALA	2.4
1	C	1	MET	2.3
1	E	364	GLY	2.3
1	F	122	ASN	2.3
1	A	427	GLU	2.3
1	E	362	SER	2.3
1	F	261	GLY	2.3
1	C	-1	SER	2.3
1	E	223	VAL	2.3
1	D	260	ASN	2.3
1	F	3	LEU	2.3
1	E	312	VAL	2.3
1	E	267	VAL	2.3
1	D	305	PRO	2.2
1	D	247	VAL	2.2
1	D	426	ASN	2.2
1	D	211	ALA	2.2
1	E	243	GLY	2.1
1	D	18	SER	2.1
1	E	292	SER	2.1
1	F	428	ASN	2.1
1	E	254	GLY	2.1
1	F	306	TRP	2.1
1	F	256	ILE	2.0
1	D	300	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	247	VAL	2.0
1	D	428	ASN	2.0
1	D	254	GLY	2.0
1	A	1	MET	2.0
1	E	365	VAL	2.0
1	E	313	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	GOL	D	503	6/6	0.87	0.22	39,44,51,52	0
4	GOL	E	503	6/6	0.87	0.20	35,38,39,43	0
4	GOL	A	503	6/6	0.91	0.25	32,40,41,41	0
3	AKG	F	502	10/10	0.92	0.17	31,35,42,45	0
3	AKG	A	502	10/10	0.92	0.17	28,34,39,42	0
3	AKG	B	502	10/10	0.92	0.16	33,38,47,49	0
3	AKG	E	502	10/10	0.92	0.18	29,34,41,42	0
4	GOL	D	504	6/6	0.93	0.13	37,44,46,46	0
2	NDP	D	501	48/48	0.93	0.17	42,52,67,69	0
3	AKG	D	502	10/10	0.94	0.19	36,43,49,53	0
3	AKG	C	502	10/10	0.94	0.16	26,32,35,36	0
4	GOL	B	503	6/6	0.94	0.16	32,35,36,37	0
2	NDP	F	501	48/48	0.95	0.17	36,45,56,59	0
2	NDP	E	501	48/48	0.96	0.13	34,45,53,60	0
2	NDP	B	501	48/48	0.97	0.13	28,38,46,48	0
2	NDP	C	501	48/48	0.97	0.13	21,28,33,39	0
2	NDP	A	501	48/48	0.98	0.11	28,35,42,43	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 AKG F 502:

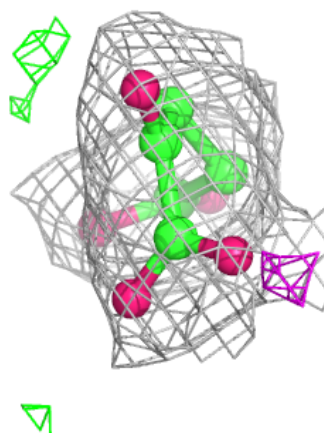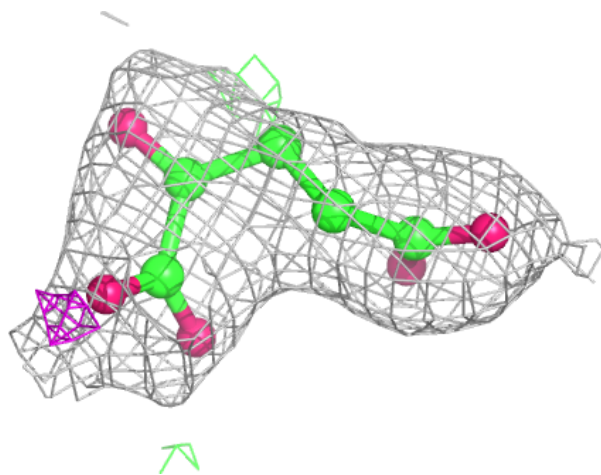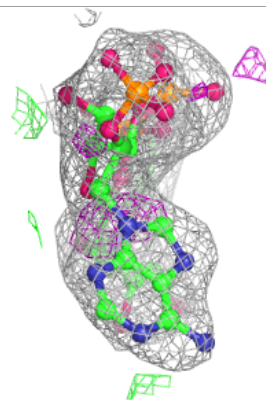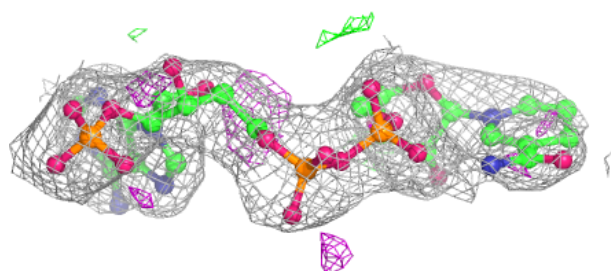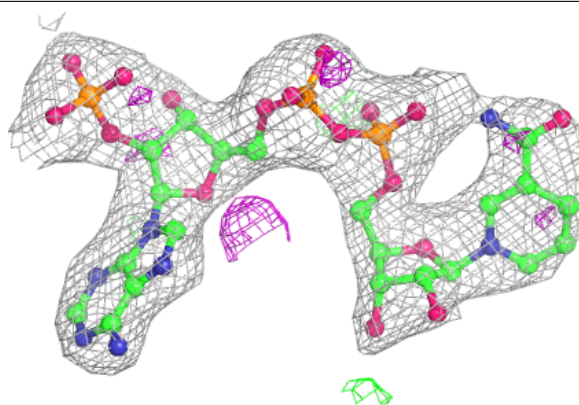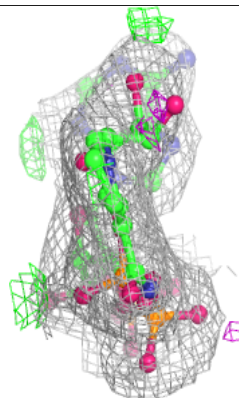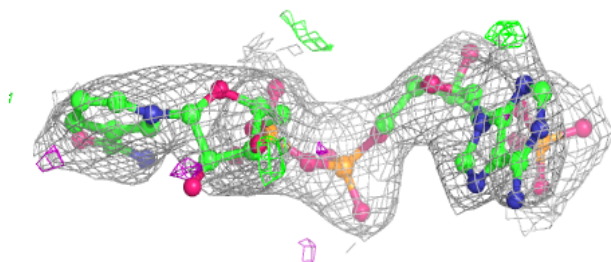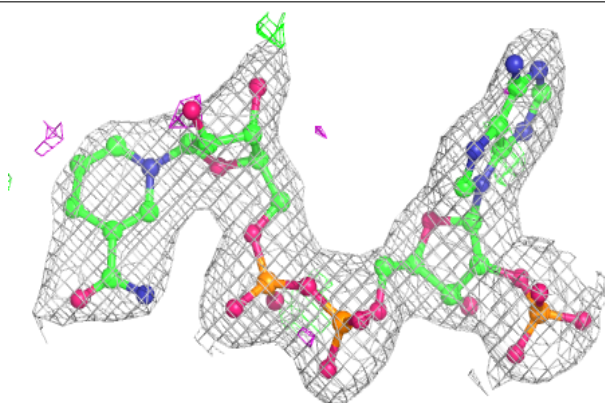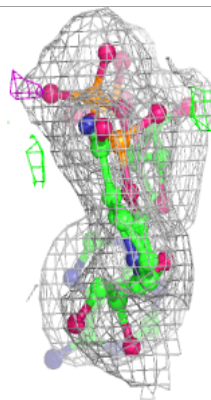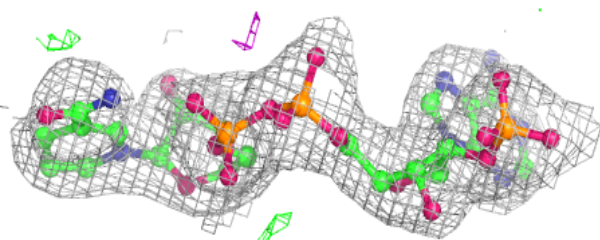$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around AKG A 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
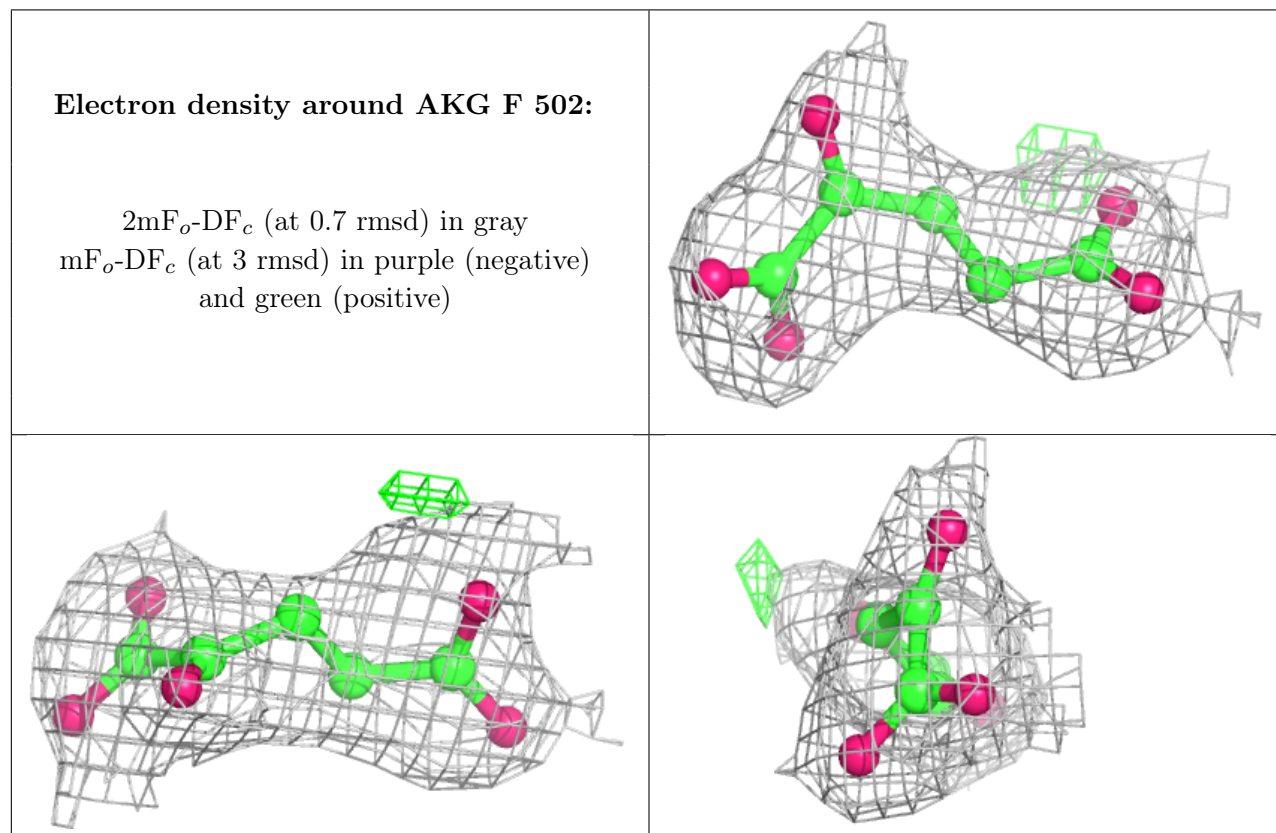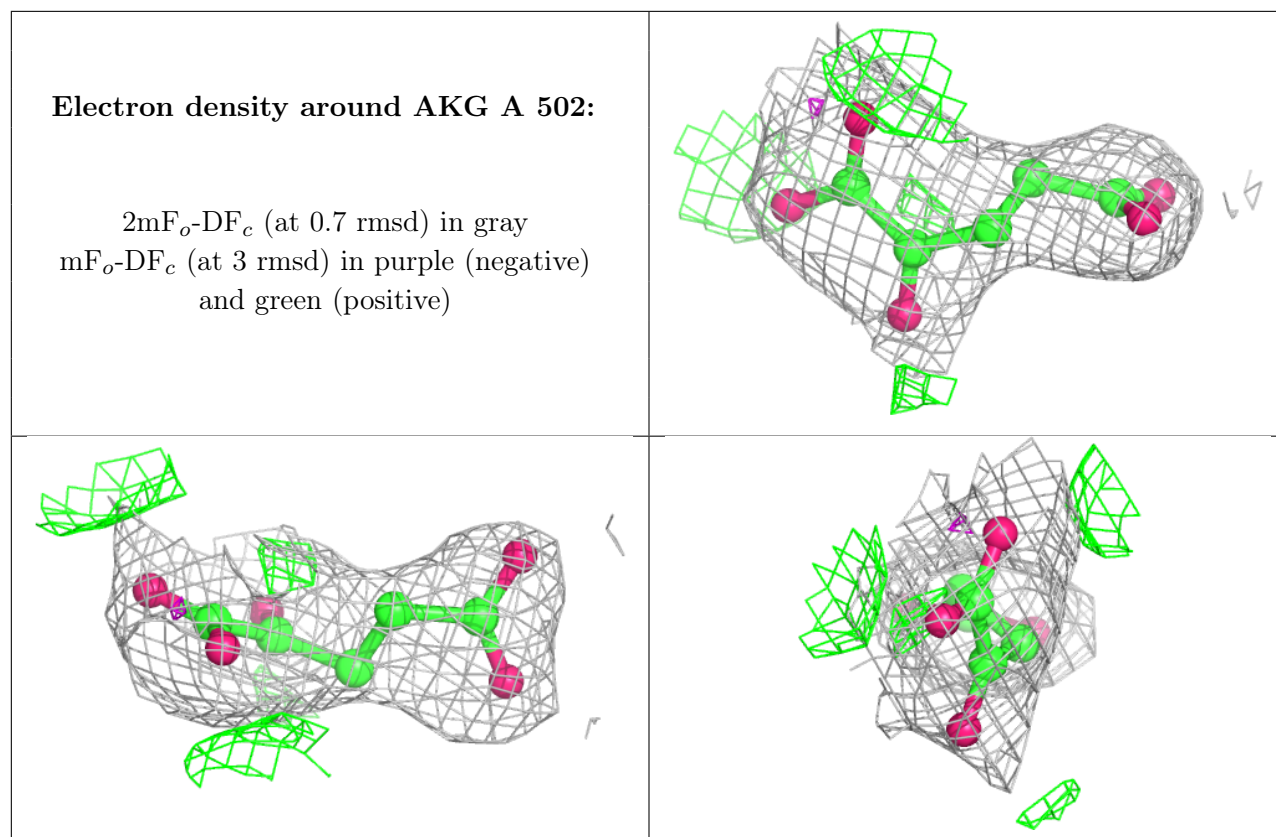
Electron density around AKG B 502:

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 AKG E 502:

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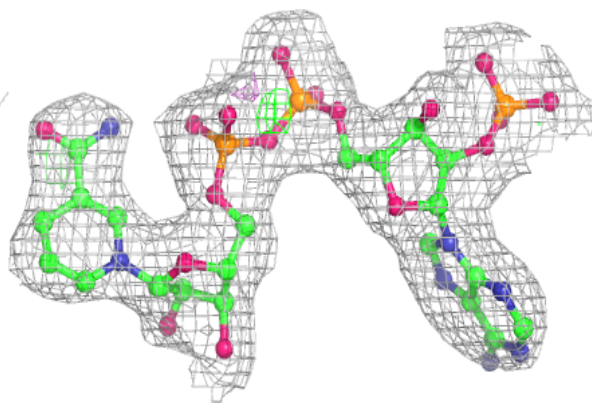and green (positive)

Electron density around NDP D 501:

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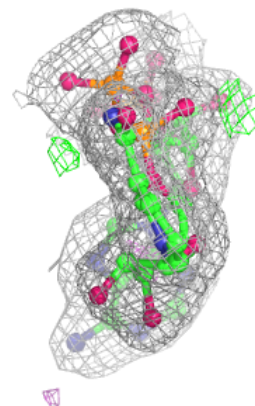mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around AKG D 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
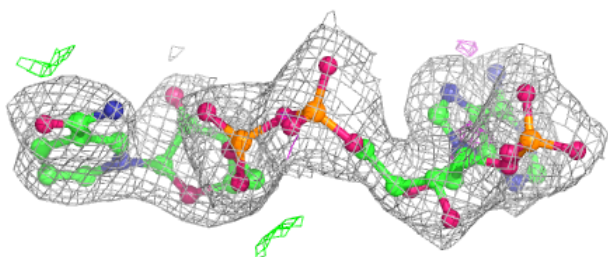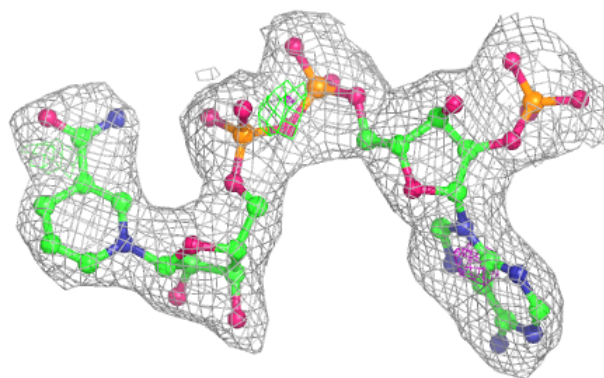and green (positive)
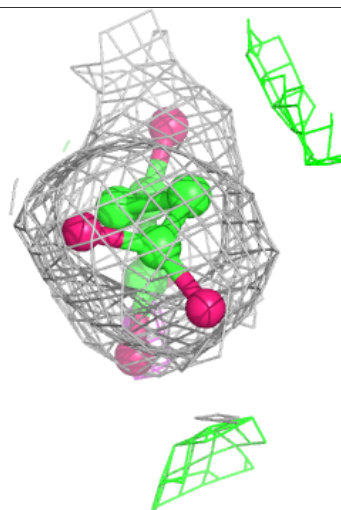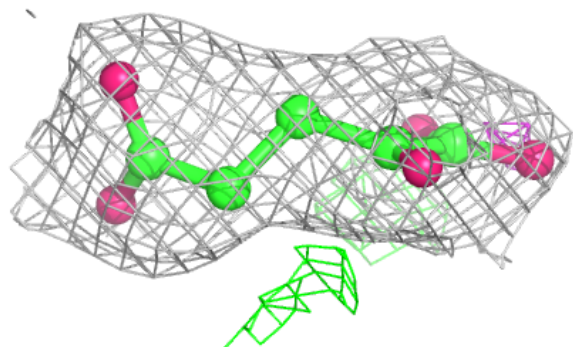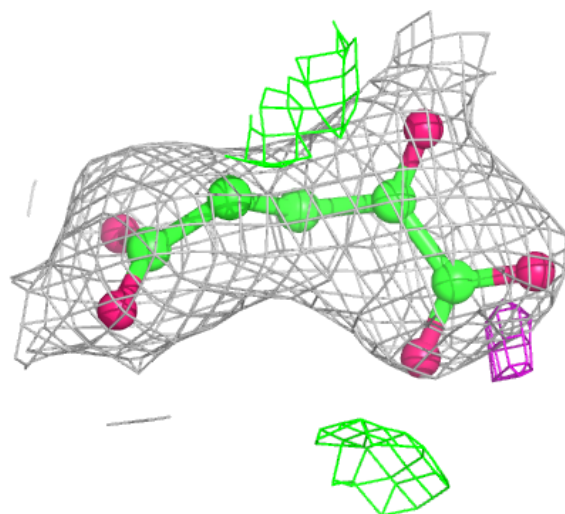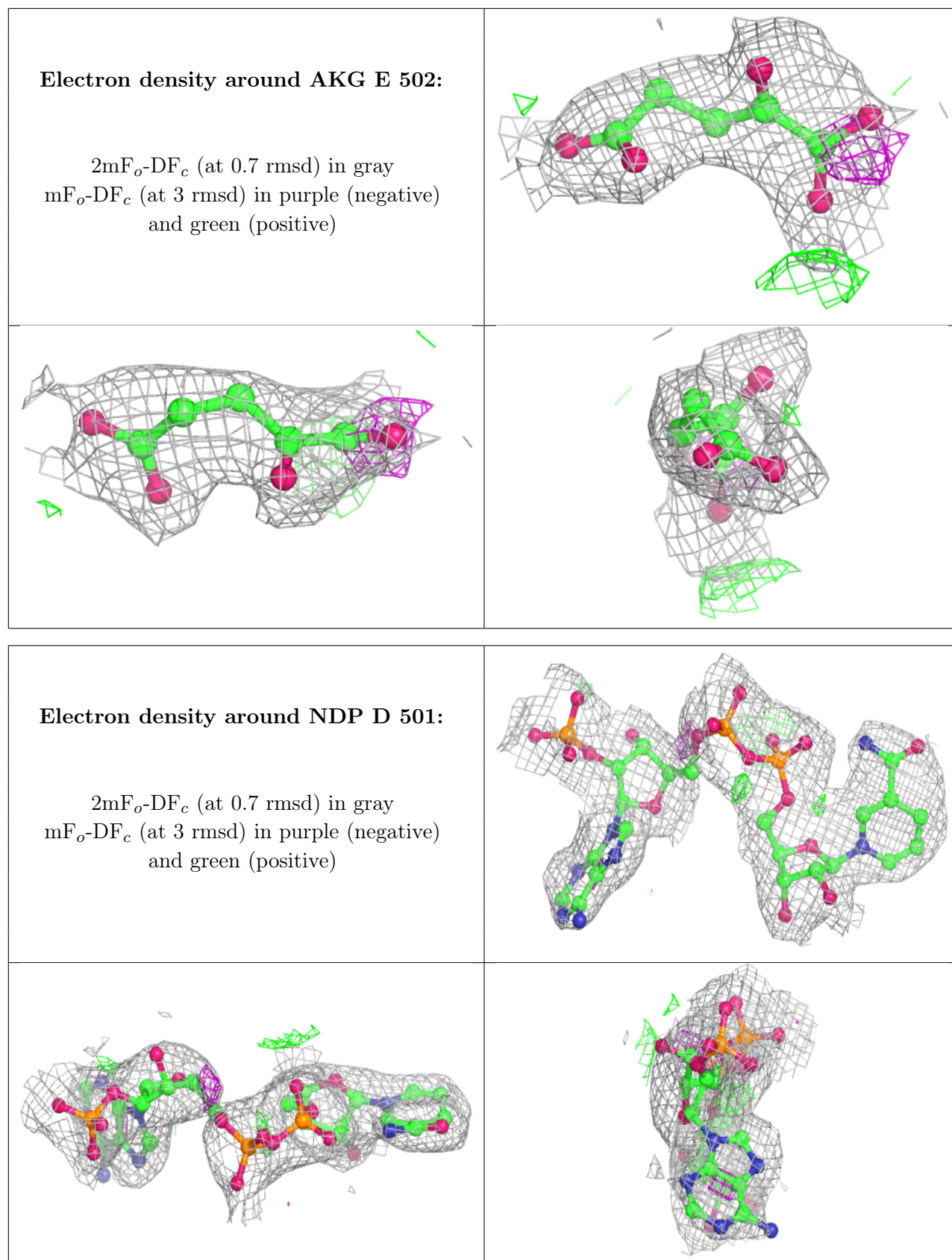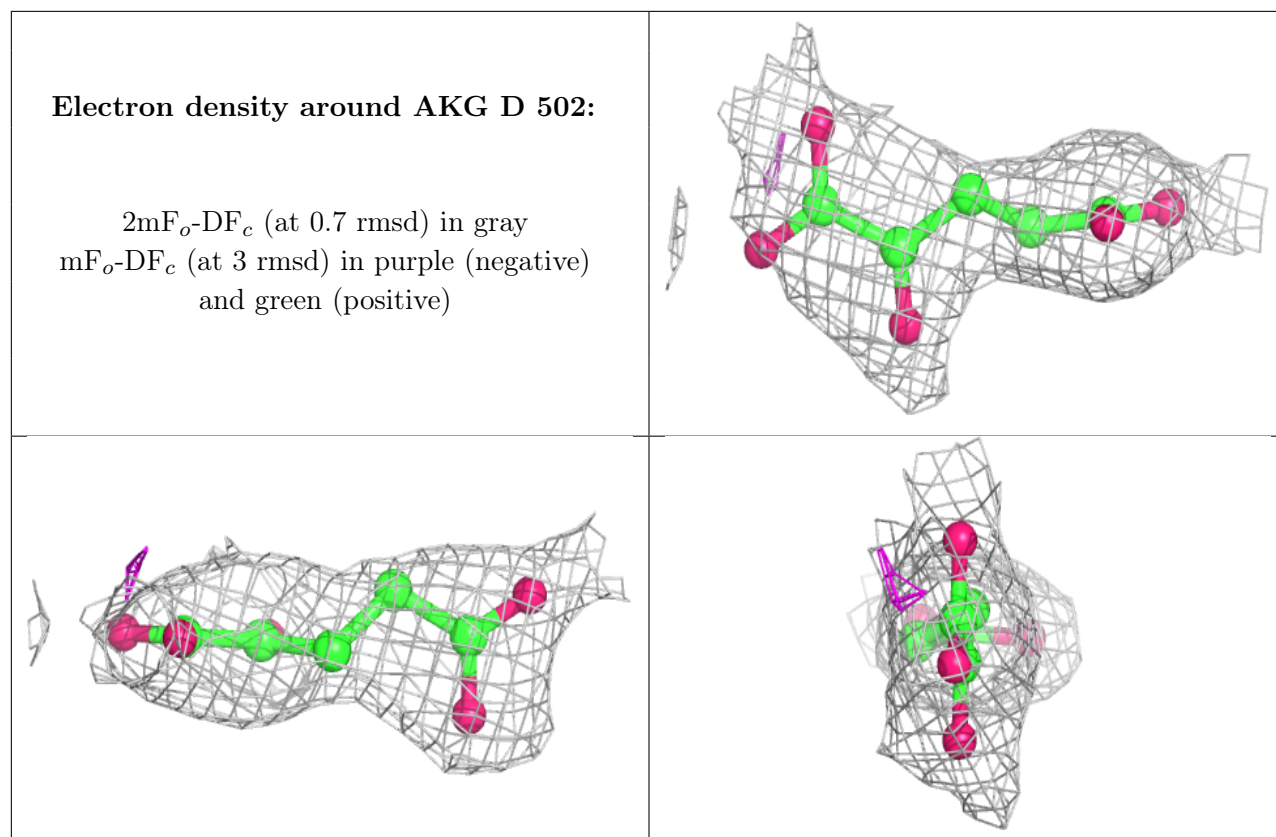
Electron density around AKG C 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
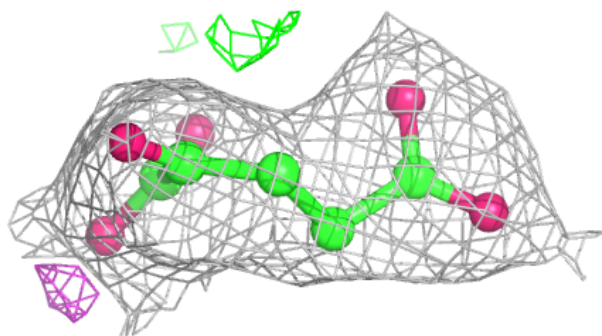
Electron density around NDP F 501:

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

Electron density around NDP E 501:

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

Electron density around NDP B 501:

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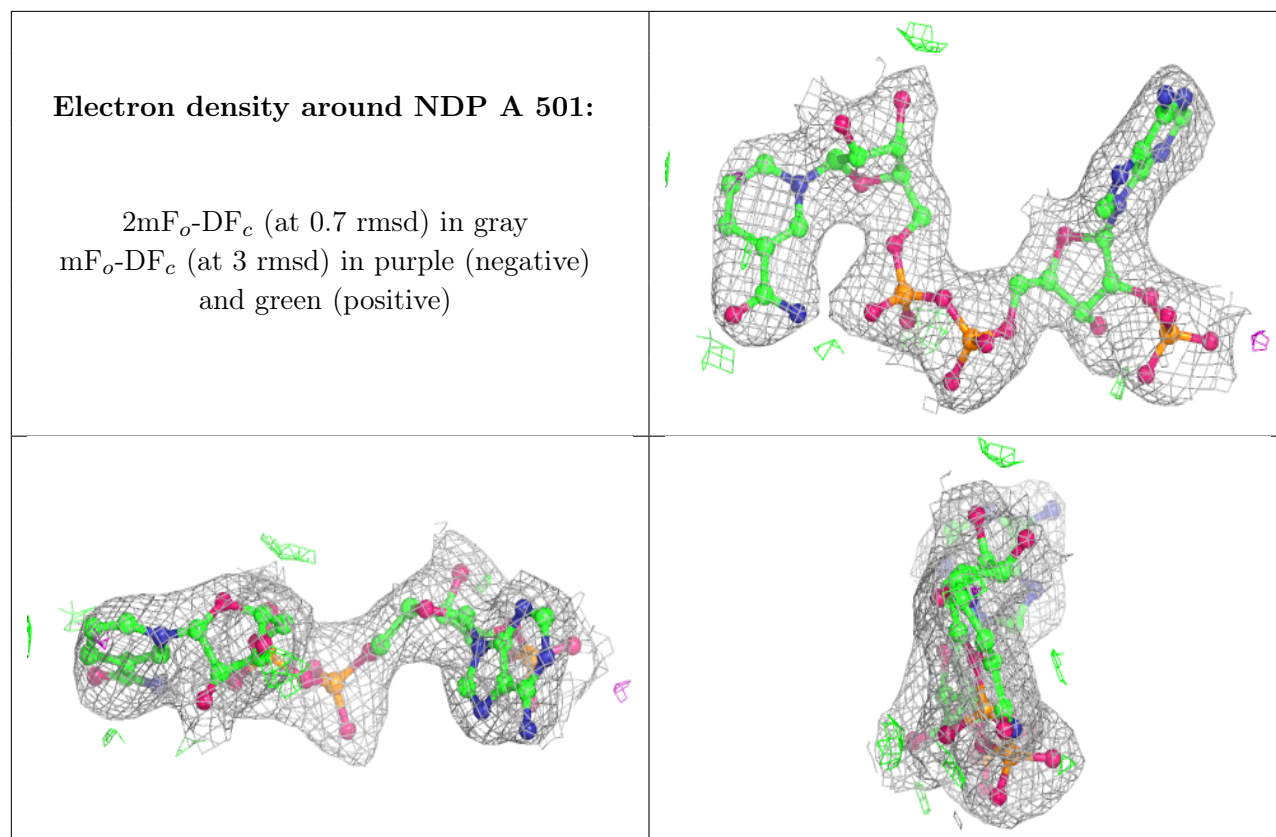mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NDP C 501:

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 NDP A 501:

$2mF_o$-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 ⓘ

There are no such residues in this entry.