wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 05:14 PM EDT

PDB ID	:	6MSO
Title	:	Crystal structure of mitochondrial fumarate hydratase from Leishmania major in a complex with inhibitor thiomalate
Authors	:	Feliciano, P.R.; Drennan, C.L.; Nonato, M.C.
Deposited on	:	2018-10-17
Resolution	:	2.05 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 (i)) were used in the production of this report:

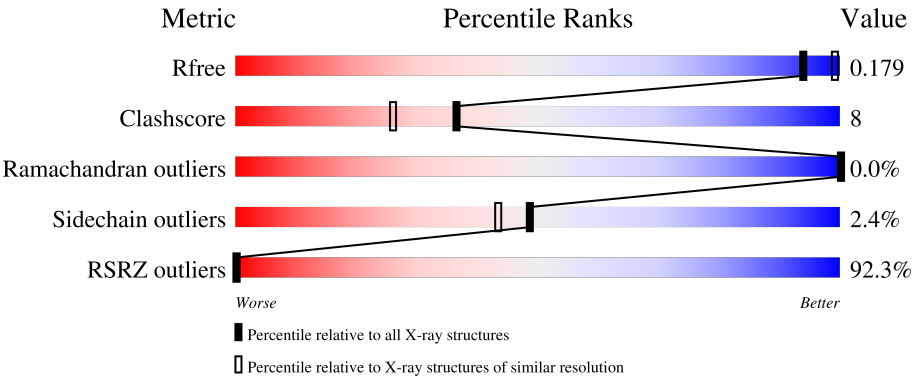
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	585	82% 81% 10% • 8%
1	B	585	82% 77% 15% • 8%
1	C	585	88% 69% 20% • 10%
1	D	585	86% 75% 16% • 9%

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	GOL	A	604	-	-	-	X
3	GOL	A	605	-	-	-	X
3	GOL	A	606	-	-	-	X
3	GOL	C	602	-	-	-	X
4	1PE	A	607	-	-	-	X
4	1PE	B	605	-	-	-	X
4	1PE	B	606	-	-	-	X
5	JYD	C	604	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17547 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 fumarate hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	3	0
			4169	2644	715	780	30			
1	B	540	Total	C	N	O	S	0	4	0
			4174	2649	712	780	33			
1	C	528	Total	C	N	O	S	0	3	0
			4055	2573	698	755	29			
1	D	531	Total	C	N	O	S	0	2	0
			4039	2562	693	755	29			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP Q4QAU9
A	-34	GLY	-	expression tag	UNP Q4QAU9
A	-33	SER	-	expression tag	UNP Q4QAU9
A	-32	SER	-	expression tag	UNP Q4QAU9
A	-31	HIS	-	expression tag	UNP Q4QAU9
A	-30	HIS	-	expression tag	UNP Q4QAU9
A	-29	HIS	-	expression tag	UNP Q4QAU9
A	-28	HIS	-	expression tag	UNP Q4QAU9
A	-27	HIS	-	expression tag	UNP Q4QAU9
A	-26	HIS	-	expression tag	UNP Q4QAU9
A	-25	SER	-	expression tag	UNP Q4QAU9
A	-24	SER	-	expression tag	UNP Q4QAU9
A	-23	GLY	-	expression tag	UNP Q4QAU9
A	-22	LEU	-	expression tag	UNP Q4QAU9
A	-21	VAL	-	expression tag	UNP Q4QAU9
A	-20	PRO	-	expression tag	UNP Q4QAU9
A	-19	ARG	-	expression tag	UNP Q4QAU9
A	-18	GLY	-	expression tag	UNP Q4QAU9
A	-17	SER	-	expression tag	UNP Q4QAU9
A	-16	HIS	-	expression tag	UNP Q4QAU9
A	-15	MET	-	expression tag	UNP Q4QAU9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ALA	-	expression tag	UNP Q4QAU9
A	-13	SER	-	expression tag	UNP Q4QAU9
A	-12	MET	-	expression tag	UNP Q4QAU9
A	-11	THR	-	expression tag	UNP Q4QAU9
A	-10	GLY	-	expression tag	UNP Q4QAU9
A	-9	GLY	-	expression tag	UNP Q4QAU9
A	-8	GLN	-	expression tag	UNP Q4QAU9
A	-7	GLN	-	expression tag	UNP Q4QAU9
A	-6	MET	-	expression tag	UNP Q4QAU9
A	-5	GLY	-	expression tag	UNP Q4QAU9
A	-4	ARG	-	expression tag	UNP Q4QAU9
A	-3	GLY	-	expression tag	UNP Q4QAU9
A	-2	SER	-	expression tag	UNP Q4QAU9
A	-1	GLU	-	expression tag	UNP Q4QAU9
A	0	PHE	-	expression tag	UNP Q4QAU9
B	-35	MET	-	initiating methionine	UNP Q4QAU9
B	-34	GLY	-	expression tag	UNP Q4QAU9
B	-33	SER	-	expression tag	UNP Q4QAU9
B	-32	SER	-	expression tag	UNP Q4QAU9
B	-31	HIS	-	expression tag	UNP Q4QAU9
B	-30	HIS	-	expression tag	UNP Q4QAU9
B	-29	HIS	-	expression tag	UNP Q4QAU9
B	-28	HIS	-	expression tag	UNP Q4QAU9
B	-27	HIS	-	expression tag	UNP Q4QAU9
B	-26	HIS	-	expression tag	UNP Q4QAU9
B	-25	SER	-	expression tag	UNP Q4QAU9
B	-24	SER	-	expression tag	UNP Q4QAU9
B	-23	GLY	-	expression tag	UNP Q4QAU9
B	-22	LEU	-	expression tag	UNP Q4QAU9
B	-21	VAL	-	expression tag	UNP Q4QAU9
B	-20	PRO	-	expression tag	UNP Q4QAU9
B	-19	ARG	-	expression tag	UNP Q4QAU9
B	-18	GLY	-	expression tag	UNP Q4QAU9
B	-17	SER	-	expression tag	UNP Q4QAU9
B	-16	HIS	-	expression tag	UNP Q4QAU9
B	-15	MET	-	expression tag	UNP Q4QAU9
B	-14	ALA	-	expression tag	UNP Q4QAU9
B	-13	SER	-	expression tag	UNP Q4QAU9
B	-12	MET	-	expression tag	UNP Q4QAU9
B	-11	THR	-	expression tag	UNP Q4QAU9
B	-10	GLY	-	expression tag	UNP Q4QAU9
B	-9	GLY	-	expression tag	UNP Q4QAU9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLN	-	expression tag	UNP Q4QAU9
B	-7	GLN	-	expression tag	UNP Q4QAU9
B	-6	MET	-	expression tag	UNP Q4QAU9
B	-5	GLY	-	expression tag	UNP Q4QAU9
B	-4	ARG	-	expression tag	UNP Q4QAU9
B	-3	GLY	-	expression tag	UNP Q4QAU9
B	-2	SER	-	expression tag	UNP Q4QAU9
B	-1	GLU	-	expression tag	UNP Q4QAU9
B	0	PHE	-	expression tag	UNP Q4QAU9
C	-35	MET	-	initiating methionine	UNP Q4QAU9
C	-34	GLY	-	expression tag	UNP Q4QAU9
C	-33	SER	-	expression tag	UNP Q4QAU9
C	-32	SER	-	expression tag	UNP Q4QAU9
C	-31	HIS	-	expression tag	UNP Q4QAU9
C	-30	HIS	-	expression tag	UNP Q4QAU9
C	-29	HIS	-	expression tag	UNP Q4QAU9
C	-28	HIS	-	expression tag	UNP Q4QAU9
C	-27	HIS	-	expression tag	UNP Q4QAU9
C	-26	HIS	-	expression tag	UNP Q4QAU9
C	-25	SER	-	expression tag	UNP Q4QAU9
C	-24	SER	-	expression tag	UNP Q4QAU9
C	-23	GLY	-	expression tag	UNP Q4QAU9
C	-22	LEU	-	expression tag	UNP Q4QAU9
C	-21	VAL	-	expression tag	UNP Q4QAU9
C	-20	PRO	-	expression tag	UNP Q4QAU9
C	-19	ARG	-	expression tag	UNP Q4QAU9
C	-18	GLY	-	expression tag	UNP Q4QAU9
C	-17	SER	-	expression tag	UNP Q4QAU9
C	-16	HIS	-	expression tag	UNP Q4QAU9
C	-15	MET	-	expression tag	UNP Q4QAU9
C	-14	ALA	-	expression tag	UNP Q4QAU9
C	-13	SER	-	expression tag	UNP Q4QAU9
C	-12	MET	-	expression tag	UNP Q4QAU9
C	-11	THR	-	expression tag	UNP Q4QAU9
C	-10	GLY	-	expression tag	UNP Q4QAU9
C	-9	GLY	-	expression tag	UNP Q4QAU9
C	-8	GLN	-	expression tag	UNP Q4QAU9
C	-7	GLN	-	expression tag	UNP Q4QAU9
C	-6	MET	-	expression tag	UNP Q4QAU9
C	-5	GLY	-	expression tag	UNP Q4QAU9
C	-4	ARG	-	expression tag	UNP Q4QAU9
C	-3	GLY	-	expression tag	UNP Q4QAU9

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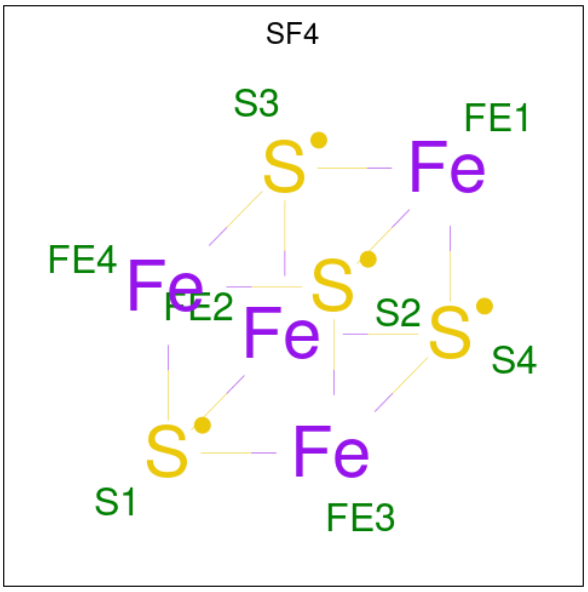
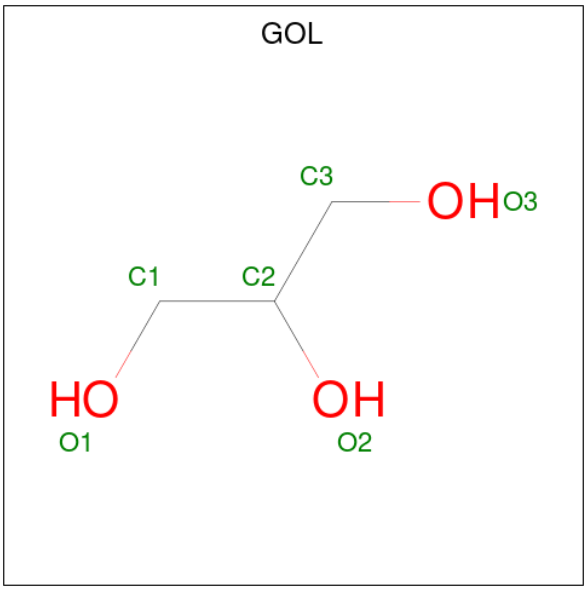
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP Q4QAU9
C	-1	GLU	-	expression tag	UNP Q4QAU9
C	0	PHE	-	expression tag	UNP Q4QAU9
D	-35	MET	-	initiating methionine	UNP Q4QAU9
D	-34	GLY	-	expression tag	UNP Q4QAU9
D	-33	SER	-	expression tag	UNP Q4QAU9
D	-32	SER	-	expression tag	UNP Q4QAU9
D	-31	HIS	-	expression tag	UNP Q4QAU9
D	-30	HIS	-	expression tag	UNP Q4QAU9
D	-29	HIS	-	expression tag	UNP Q4QAU9
D	-28	HIS	-	expression tag	UNP Q4QAU9
D	-27	HIS	-	expression tag	UNP Q4QAU9
D	-26	HIS	-	expression tag	UNP Q4QAU9
D	-25	SER	-	expression tag	UNP Q4QAU9
D	-24	SER	-	expression tag	UNP Q4QAU9
D	-23	GLY	-	expression tag	UNP Q4QAU9
D	-22	LEU	-	expression tag	UNP Q4QAU9
D	-21	VAL	-	expression tag	UNP Q4QAU9
D	-20	PRO	-	expression tag	UNP Q4QAU9
D	-19	ARG	-	expression tag	UNP Q4QAU9
D	-18	GLY	-	expression tag	UNP Q4QAU9
D	-17	SER	-	expression tag	UNP Q4QAU9
D	-16	HIS	-	expression tag	UNP Q4QAU9
D	-15	MET	-	expression tag	UNP Q4QAU9
D	-14	ALA	-	expression tag	UNP Q4QAU9
D	-13	SER	-	expression tag	UNP Q4QAU9
D	-12	MET	-	expression tag	UNP Q4QAU9
D	-11	THR	-	expression tag	UNP Q4QAU9
D	-10	GLY	-	expression tag	UNP Q4QAU9
D	-9	GLY	-	expression tag	UNP Q4QAU9
D	-8	GLN	-	expression tag	UNP Q4QAU9
D	-7	GLN	-	expression tag	UNP Q4QAU9
D	-6	MET	-	expression tag	UNP Q4QAU9
D	-5	GLY	-	expression tag	UNP Q4QAU9
D	-4	ARG	-	expression tag	UNP Q4QAU9
D	-3	GLY	-	expression tag	UNP Q4QAU9
D	-2	SER	-	expression tag	UNP Q4QAU9
D	-1	GLU	-	expression tag	UNP Q4QAU9
D	0	PHE	-	expression tag	UNP Q4QAU9

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



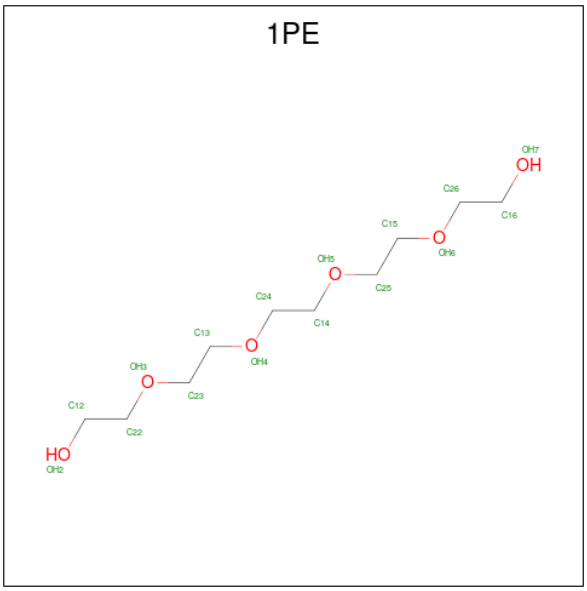
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0

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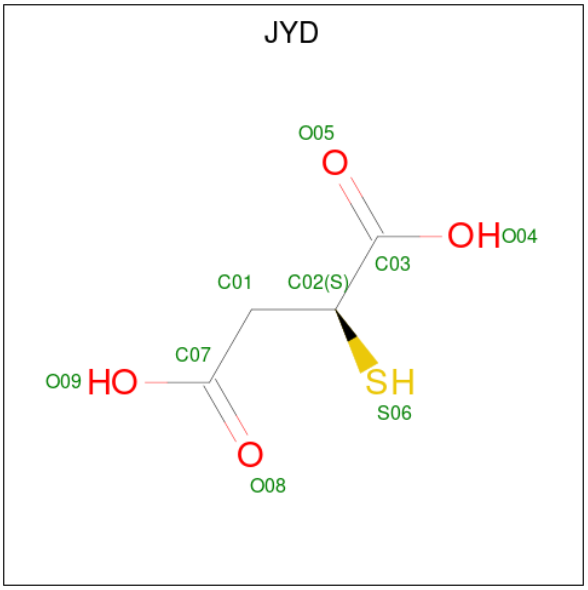
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 13 8 5	0	0
4	B	1	Total C O 10 6 4	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 10 6 4	0	0
4	C	1	Total C O 10 6 4	0	0
4	D	1	Total C O 16 10 6	0	0

- Molecule 5 is (2S)-2-sulfanylbutanedioic acid (three-letter code: JYD) (formula: $C_4H_6O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O S 18 8 8 2	0	1
5	B	1	Total C O S 18 8 8 2	0	1
5	C	1	Total C O S 9 4 4 1	0	0
5	D	1	Total C O S 9 4 4 1	0	0

- Molecule 6 is water.

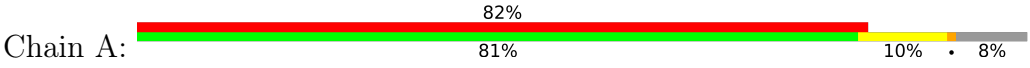
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	251	Total O 252 252	0	1
6	B	282	Total O 282 282	0	0
6	C	166	Total O 167 167	0	1
6	D	168	Total O 169 169	0	1

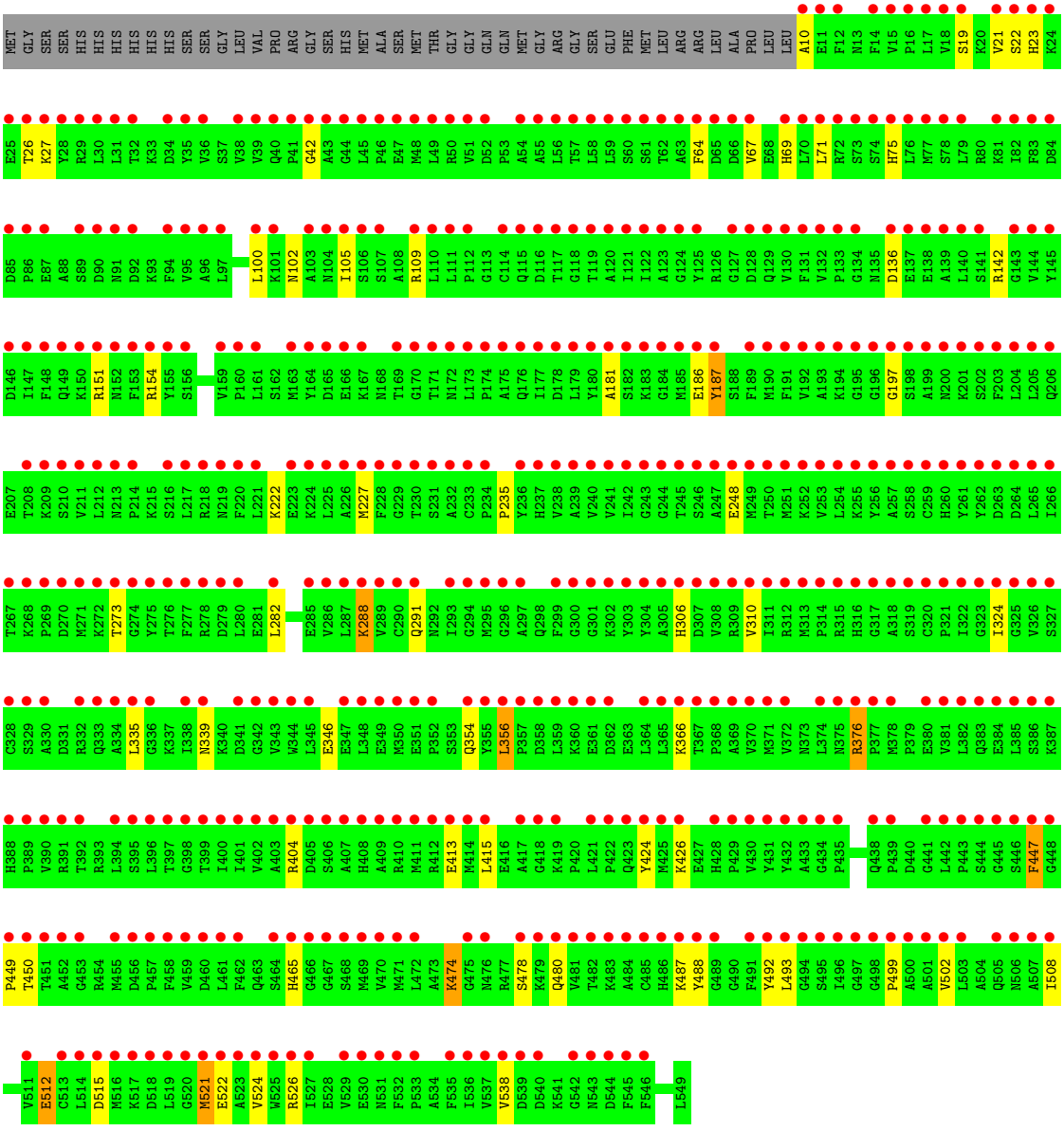
3 Residue-property plots (i)

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: fumarate hydratase

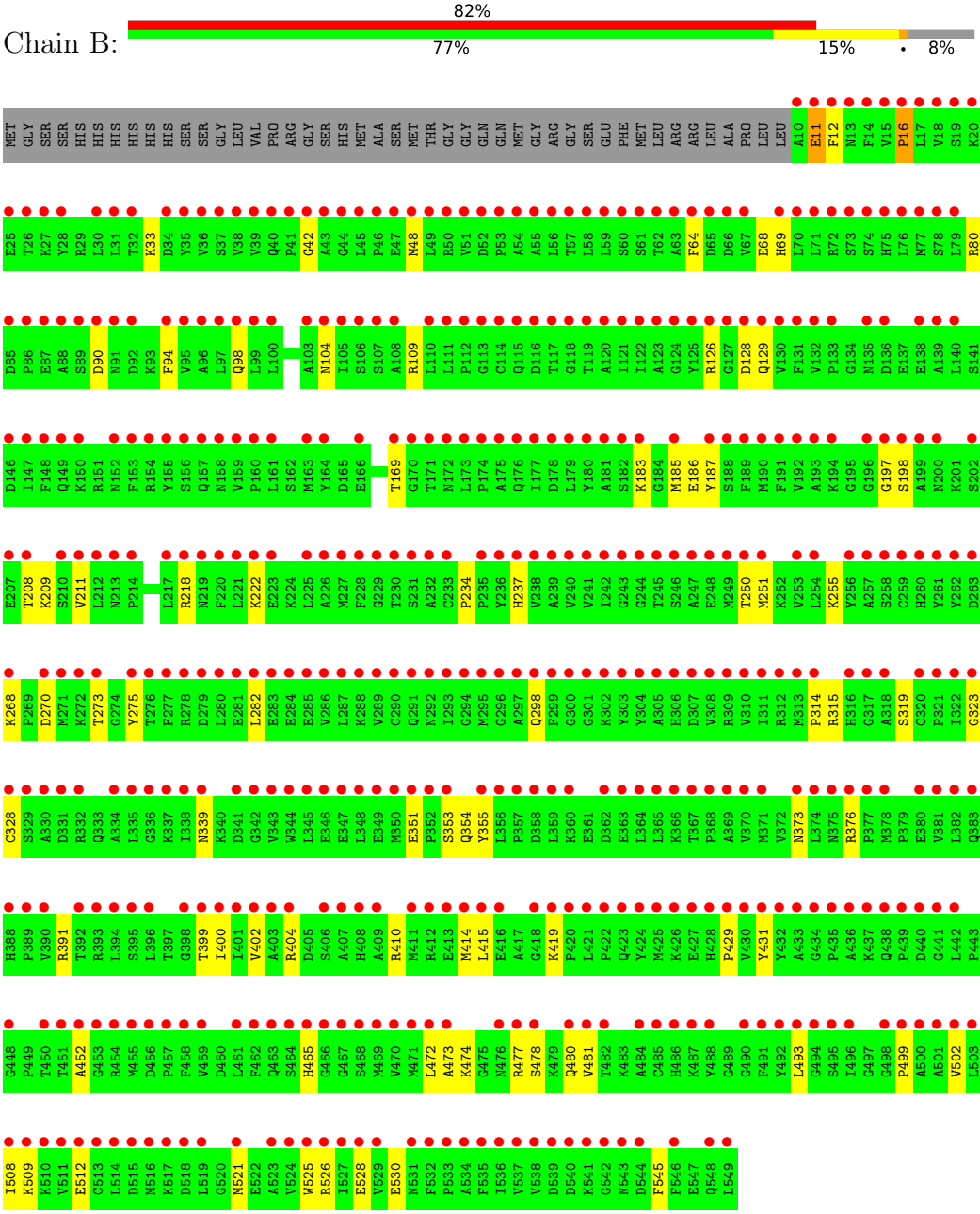
Chain A:





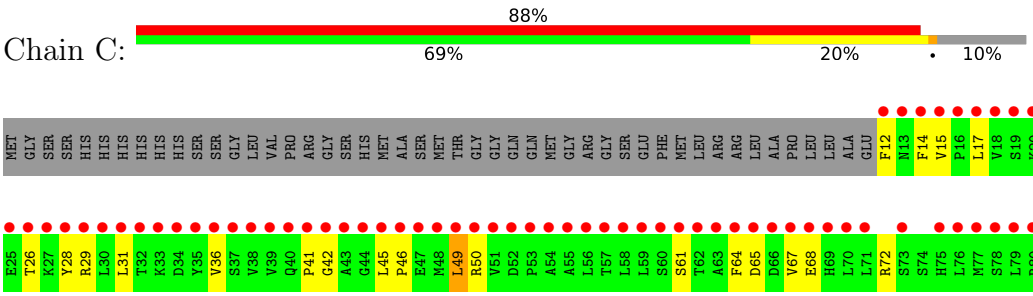
• Molecule 1: fumarate hydratase

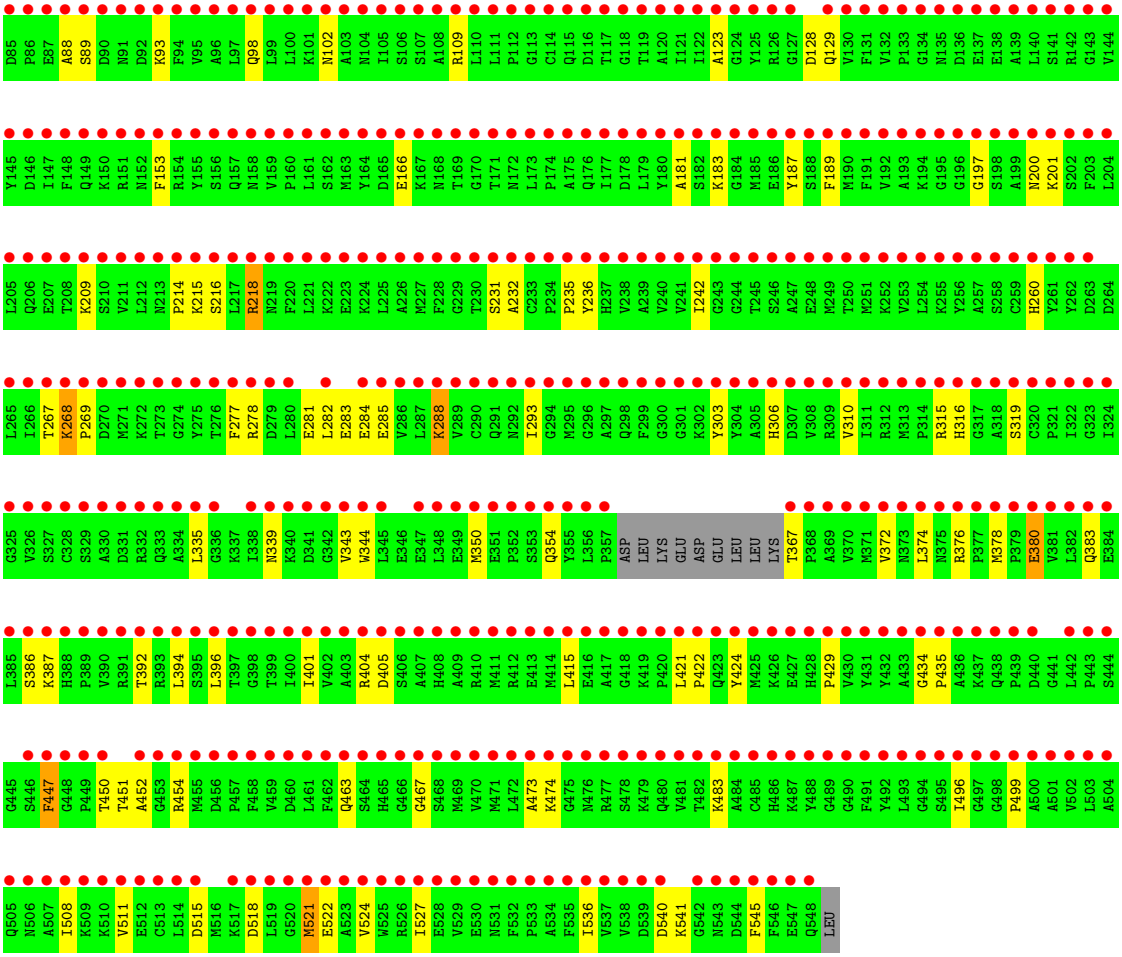
Chain B:



• Molecule 1: fumarate hydratase

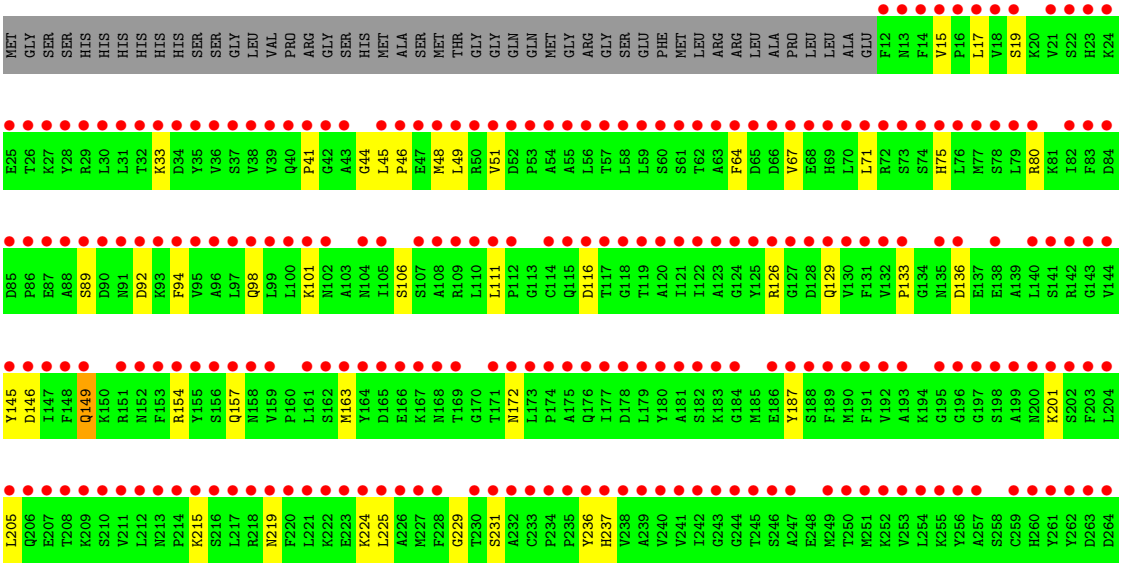
Chain C:

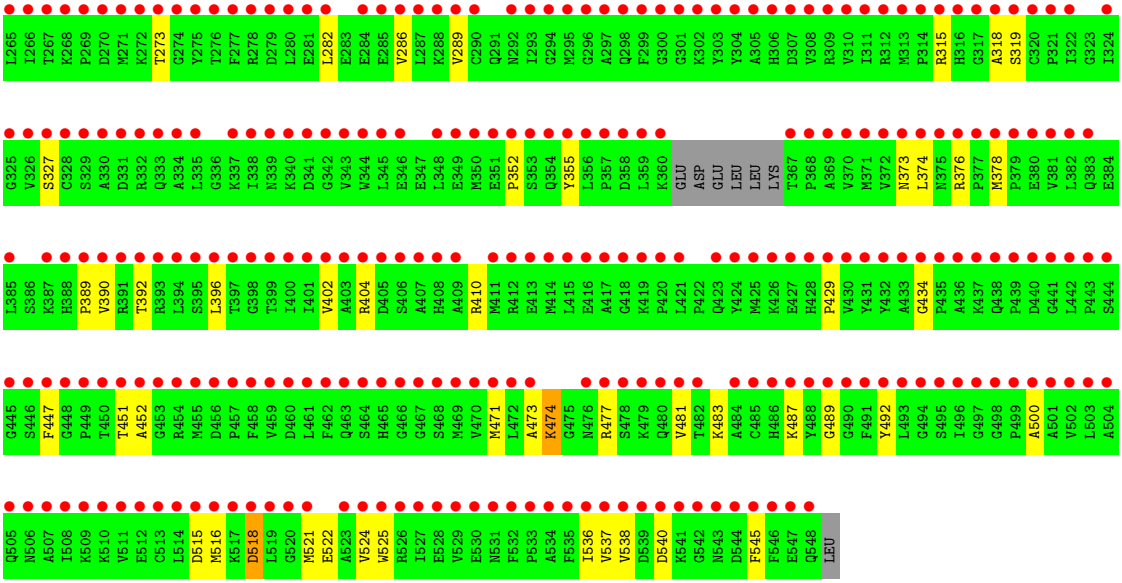




• Molecule 1: fumarate hydratase

Chain D:




L265 I266 T267 K268 P269 D270 M271 K272 T273 G274 Y275 T276 P277 R278 D279 L280 E281 L282 E283 E284 E285 V286 L287 K288 V289 C290 Q291 N292 I293 G294 M295 G296 A297 Q298 P299 G300 G301 K302 Y303 Y304 A305 H306 D307 V308 R309 V310 I311 R312 M313 P314 R315 H316 G317 A318 S319 C320 P321 I322 G323 I324
G325 V326 S327 C328 S329 A330 D331 R332 Q333 A334 L335 G336 K337 I338 N339 K340 D341 G342 V343 W344 L345 E346 E347 L348 E349 M350 E351 P352 S353 Q354 Y355 L356 P357 D358 L359 K360 GLU ASP GLU LEU LEU LYS T367 P368 A369 V370 M371 V372 N373 L374 N375 R376 P377 M378 P379 E380 V381 L382 Q383 E384
L385 S386 K387 H388 P389 V390 R391 T392 R393 L394 S395 L396 T397 G398 T399 I400 I401 V402 A403 R404 D405 S406 A407 H408 A409 R410 M411 R412 E413 M414 L415 E416 A417 G418 K419 P420 L421 P422 Q423 Y424 M425 K426 E427 H428 P429 V430 Y431 Y432 A433 G434 P435 A436 K437 Q438 P439 D440 G441 L442 P443 S444
G445 S446 F447 G448 P449 T450 T451 A452 G453 R454 M455 D456 P457 F458 V459 D460 L461 F462 Q463 S464 H465 G466 G467 S468 M469 V470 M471 L472 A473 K474 G475 N476 R477 S478 K479 Q480 V481 T482 K483 A484 C485 H486 K487 Y488 G489 G490 F491 Y492 L493 G494 S495 T496 G497 G498 P499 A500 A501 V502 L503 A504
Q505 N506 A507 I508 K509 K510 V511 E512 C513 L514 D515 M516 K517 D518 L519 G520 M521 E522 A523 V524 W525 R526 I527 E528 V529 E530 N531 F532 P533 A534 F535 I536 V537 V538 D539 D540 K541 G542 N543 D544 F545 F546 E547 Q548 LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.74Å 138.44Å 138.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.05 48.88 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.88-2.05) 98.1 (48.88-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	341.80 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.159 , 0.204 0.145 , 0.179	Depositor DCC
R_{free} test set	9057 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.418 for -h,-l,-k 0.409 for -h,l,k 0.448 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17547	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SF4, JYD, 1PE

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	0.45	0/4259	0.63	0/5761
1	B	0.44	0/4264	0.62	0/5768
1	C	0.41	0/4144	0.63	1/5609 (0.0%)
1	D	0.40	0/4128	0.60	0/5595
All	All	0.43	0/16795	0.62	1/22733 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	49	LEU	CB-CG-CD1	-5.24	102.09	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4169	0	4113	46	0
1	B	4174	0	4120	62	0
1	C	4055	0	3975	88	0
1	D	4039	0	3915	71	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8	0	0	0	0
2	D	8	0	0	0	0
3	A	30	0	37	3	0
3	B	12	0	15	1	0
3	C	6	0	8	3	0
4	A	40	0	50	4	0
4	B	23	0	29	3	0
4	C	27	0	33	4	0
4	D	16	0	22	4	0
5	A	18	0	0	4	0
5	B	18	0	0	2	0
5	C	9	0	0	2	0
5	D	9	0	0	1	0
6	A	252	0	0	3	0
6	B	282	0	0	8	0
6	C	167	0	0	5	0
6	D	169	0	0	5	0
All	All	17547	0	16317	259	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 8.

The worst 5 of 259 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:GLU:HG2	4:A:610:1PE:H152	1.39	1.02
1:C:267:THR:O	1:C:268:LYS:HD2	1.62	1.00
1:B:391:ARG:NH2	6:B:701:HOH:O	2.00	0.91
1:C:521:MET:HE2	1:C:522:GLU:HG2	1.58	0.85
1:A:42:GLY:H	1:B:42:GLY:H	1.23	0.84

There are no symmetry-related clashes.

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	Percentiles
1	A	541/585 (92%)	523 (97%)	17 (3%)	1 (0%)	47 39
1	B	542/585 (93%)	525 (97%)	17 (3%)	0	100 100
1	C	527/585 (90%)	506 (96%)	21 (4%)	0	100 100
1	D	529/585 (90%)	509 (96%)	20 (4%)	0	100 100
All	All	2139/2340 (91%)	2063 (96%)	75 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	LYS

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	445/491 (91%)	435 (98%)	10 (2%)	52 46
1	B	446/491 (91%)	437 (98%)	9 (2%)	55 51
1	C	428/491 (87%)	412 (96%)	16 (4%)	34 27
1	D	421/491 (86%)	410 (97%)	11 (3%)	46 40
All	All	1740/1964 (89%)	1694 (97%)	46 (3%)	49 40

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	380[A]	GLU
1	D	15	VAL
1	C	380[B]	GLU
1	C	518	ASP
1	D	136	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	C	602	-	5,5,5	0.90	0	5,5,5	1.05	0
2	SF4	C	601	1,5	0,12,12	-	-	-		
5	JYD	A	608[B]	2	6,8,8	1.15	0	6,10,10	1.47	1 (16%)
2	SF4	A	601	1,5	0,12,12	-	-	-		
3	GOL	B	603	-	5,5,5	1.19	1 (20%)	5,5,5	1.09	0
3	GOL	A	606	-	5,5,5	1.15	1 (20%)	5,5,5	1.00	0
5	JYD	D	602	2	6,8,8	1.02	0	6,10,10	1.92	3 (50%)
4	1PE	A	610	-	9,9,15	0.36	0	8,8,14	0.35	0
2	SF4	B	601	1,5	0,12,12	-	-	-		
4	1PE	C	606	-	9,9,15	0.26	0	8,8,14	0.50	0
5	JYD	B	604[A]	2	6,8,8	1.10	0	6,10,10	1.30	0
5	JYD	C	604	2	6,8,8	1.14	0	6,10,10	1.11	0
5	JYD	A	608[A]	2	6,8,8	1.09	0	6,10,10	1.34	0
3	GOL	A	605	-	5,5,5	1.30	1 (20%)	5,5,5	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	B	602	-	5,5,5	0.84	0	5,5,5	1.56	1 (20%)
5	JYD	B	604[B]	2	6,8,8	1.13	0	6,10,10	1.18	0
4	1PE	A	607	-	6,6,15	0.50	0	5,5,14	0.38	0
2	SF4	D	601	1,5	0,12,12	-	-	-		
4	1PE	D	603	-	15,15,15	0.55	0	14,14,14	0.39	0
3	GOL	A	602	-	5,5,5	1.72	1 (20%)	5,5,5	1.08	1 (20%)
4	1PE	C	603	-	6,6,15	0.50	0	5,5,14	0.37	0
4	1PE	A	611	-	9,9,15	0.28	0	8,8,14	0.39	0
3	GOL	A	604	-	5,5,5	1.16	1 (20%)	5,5,5	1.10	0
4	1PE	C	605	-	9,9,15	0.27	0	8,8,14	0.50	0
4	1PE	B	606	-	9,9,15	0.29	0	8,8,14	0.41	0
4	1PE	A	609	-	12,12,15	0.51	0	11,11,14	0.60	0
3	GOL	A	603	-	5,5,5	1.30	1 (20%)	5,5,5	0.93	0
4	1PE	B	605	-	12,12,15	0.55	0	11,11,14	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	602	-	-	2/4/4/4	-
2	SF4	C	601	1,5	-	-	0/6/5/5
5	JYD	A	608[B]	2	-	1/6/8/8	-
2	SF4	A	601	1,5	-	-	0/6/5/5
3	GOL	B	603	-	-	0/4/4/4	-
3	GOL	A	606	-	-	2/4/4/4	-
5	JYD	D	602	2	-	2/6/8/8	-
4	1PE	A	610	-	-	5/7/7/13	-
4	1PE	C	606	-	-	3/7/7/13	-
5	JYD	B	604[A]	2	-	1/6/8/8	-
5	JYD	C	604	2	-	2/6/8/8	-
2	SF4	B	601	1,5	-	-	0/6/5/5
3	GOL	A	605	-	-	2/4/4/4	-
3	GOL	B	602	-	-	4/4/4/4	-
5	JYD	B	604[B]	2	-	2/6/8/8	-
4	1PE	A	607	-	-	1/4/4/13	-
2	SF4	D	601	1,5	-	-	0/6/5/5
4	1PE	D	603	-	-	11/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	602	-	-	0/4/4/4	-
4	1PE	C	603	-	-	4/4/4/13	-
3	GOL	A	603	-	-	2/4/4/4	-
4	1PE	A	611	-	-	5/7/7/13	-
3	GOL	A	604	-	-	4/4/4/4	-
4	1PE	C	605	-	-	4/7/7/13	-
4	1PE	B	606	-	-	4/7/7/13	-
4	1PE	A	609	-	-	7/10/10/13	-
5	JYD	A	608[A]	2	-	1/6/8/8	-
4	1PE	B	605	-	-	3/10/10/13	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	GOL	O2-C2	-3.33	1.33	1.43
3	A	605	GOL	O2-C2	-2.77	1.35	1.43
3	A	603	GOL	O2-C2	-2.70	1.35	1.43
3	B	603	GOL	O2-C2	-2.32	1.36	1.43
3	A	606	GOL	O2-C2	-2.10	1.37	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	602	JYD	O09-C07-C01	2.64	122.54	114.07
3	B	602	GOL	C3-C2-C1	-2.63	101.50	111.70
5	D	602	JYD	O08-C07-C01	-2.47	114.89	122.80
5	D	602	JYD	O04-C03-C02	2.30	120.47	114.03
3	A	602	GOL	C3-C2-C1	-2.04	103.76	111.70

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	GOL	O1-C1-C2-C3
3	A	604	GOL	O1-C1-C2-C3
3	A	606	GOL	C1-C2-C3-O3
3	C	602	GOL	O1-C1-C2-C3
5	A	608[A]	JYD	C07-C01-C02-S06

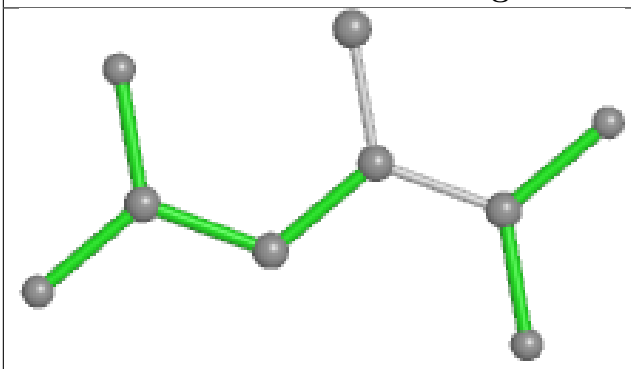
There are no ring outliers.

20 monomers are involved in 31 short contacts:

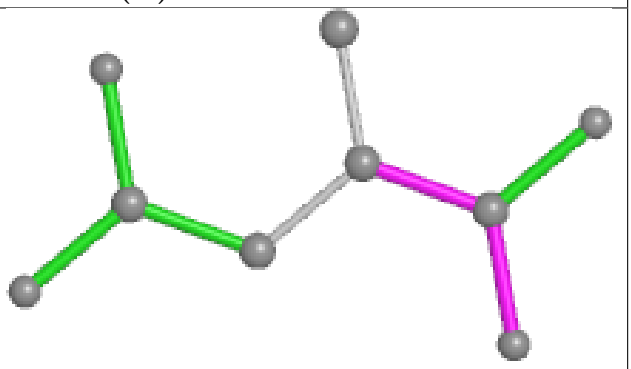
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	GOL	3	0
5	A	608[B]	JYD	3	0
5	D	602	JYD	1	0
4	A	610	1PE	1	0
4	C	606	1PE	1	0
5	B	604[A]	JYD	1	0
5	C	604	JYD	2	0
5	A	608[A]	JYD	1	0
3	B	602	GOL	1	0
5	B	604[B]	JYD	1	0
4	D	603	1PE	4	0
3	A	602	GOL	1	0
4	C	603	1PE	1	0
4	A	611	1PE	1	0
3	A	604	GOL	1	0
4	C	605	1PE	2	0
4	B	606	1PE	1	0
4	A	609	1PE	2	0
3	A	603	GOL	1	0
4	B	605	1PE	2	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.

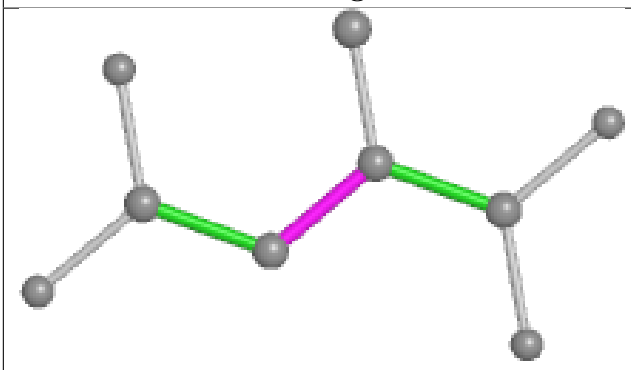
Ligand JYD A 608 (B)



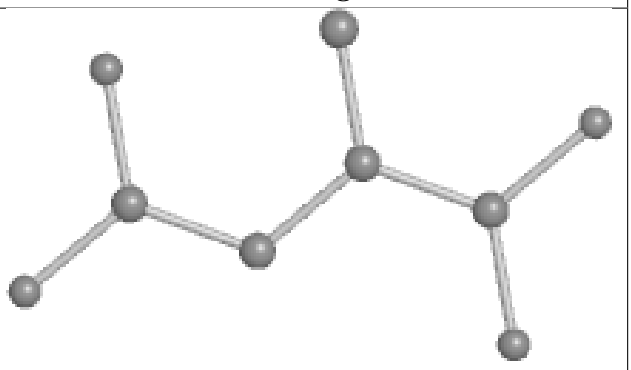
Bond lengths



Bond angles

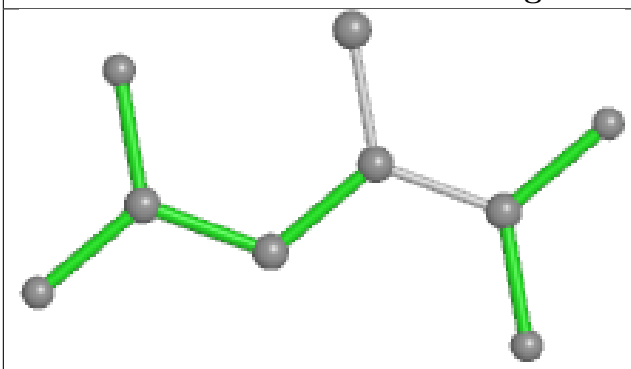


Torsions



Rings

Ligand JYD D 602



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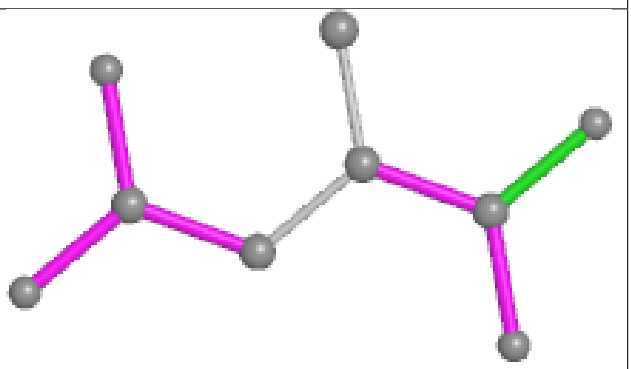
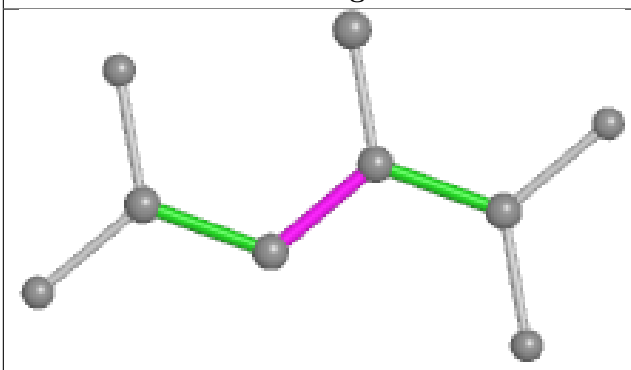


Bond angles



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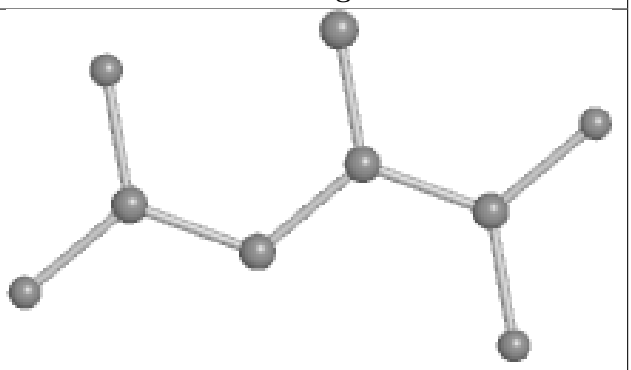
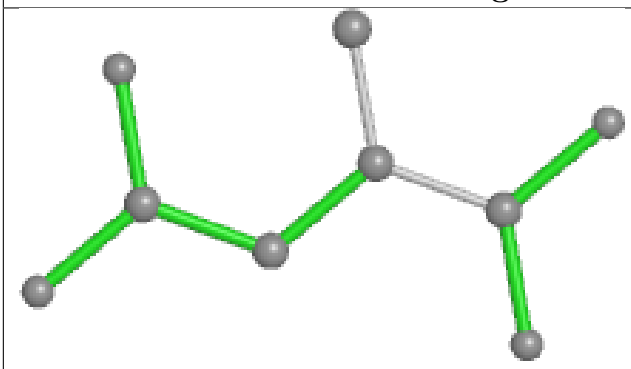
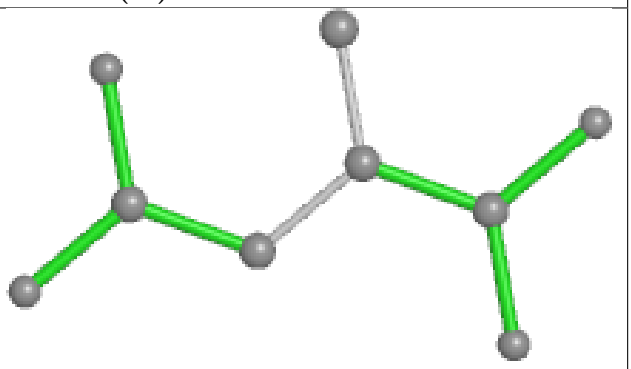


Rings

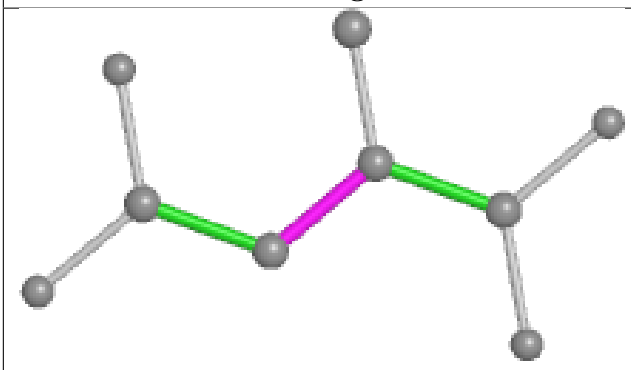
Ligand JYD B 604 (A)



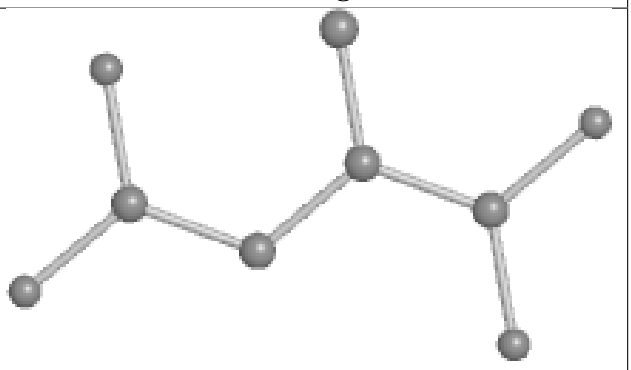
Bond lengths



Bond angles

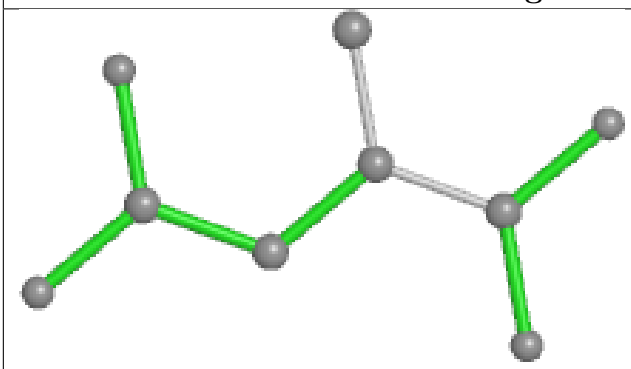


Torsions

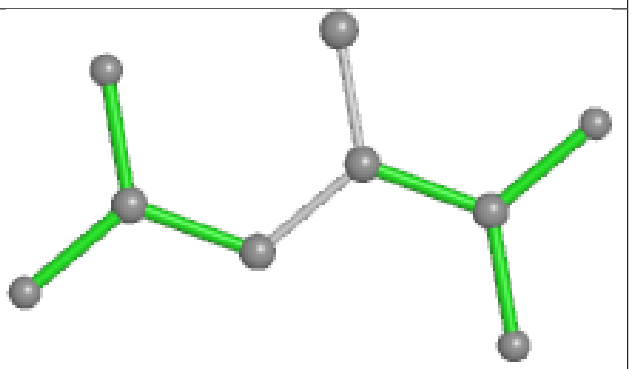


Rings

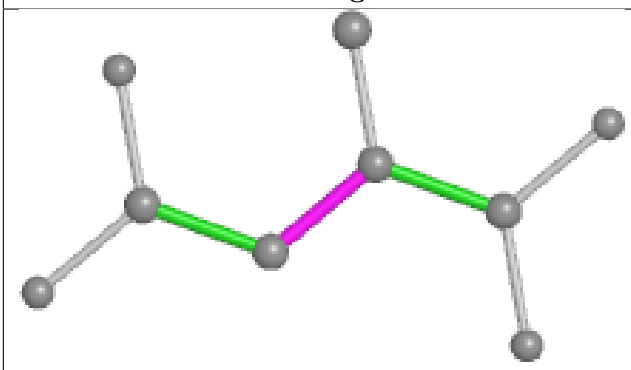
Ligand JYD C 604



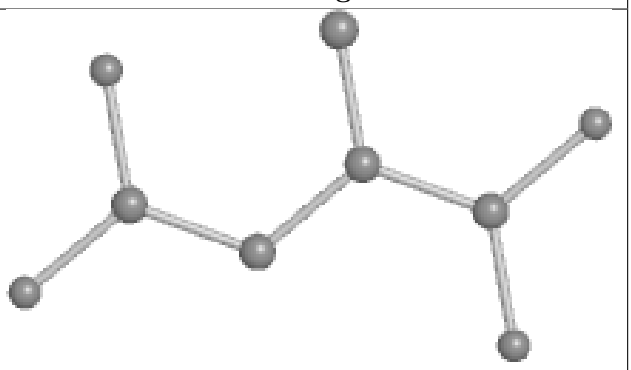
Bond lengths



Bond angles

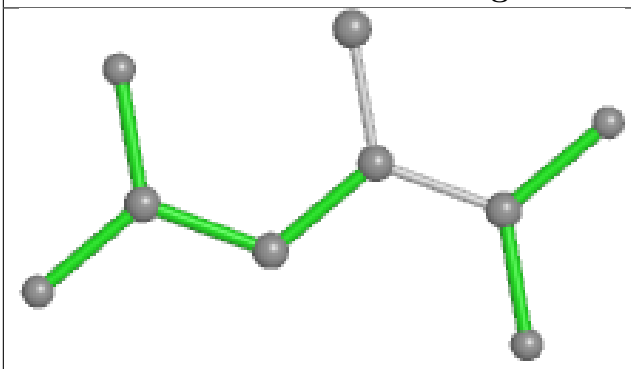


Torsions

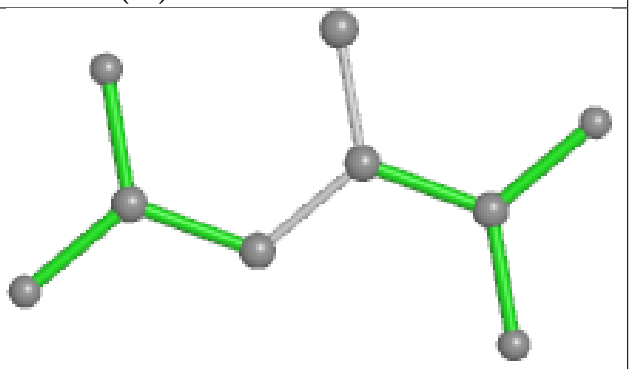


Rings

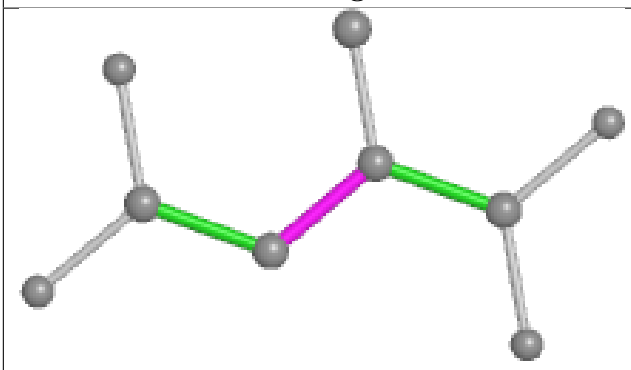
Ligand JYD A 608 (A)



Bond lengths



Bond angles



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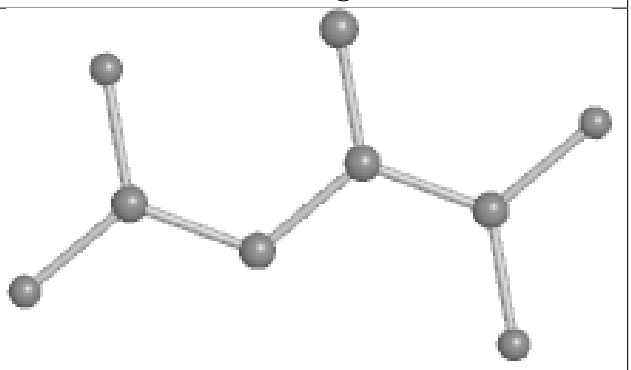
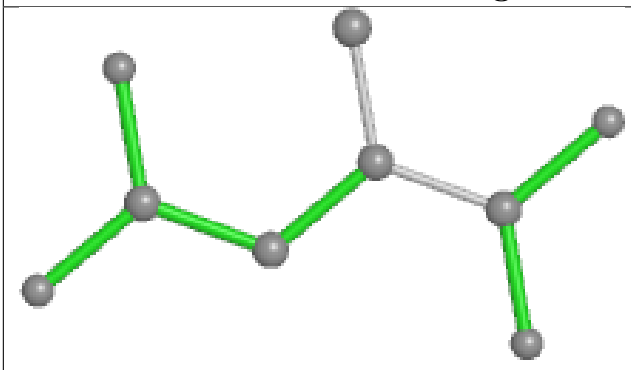
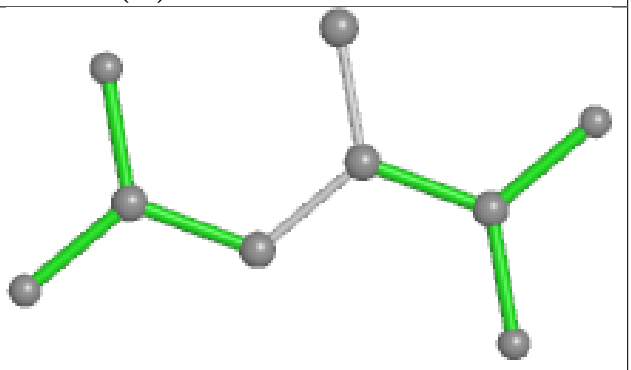


Rings

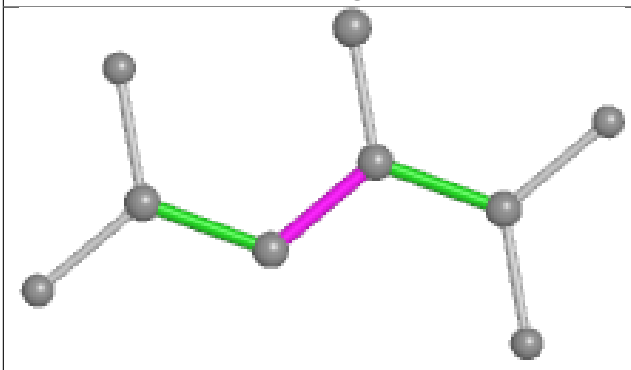
Ligand JYD B 604 (B)



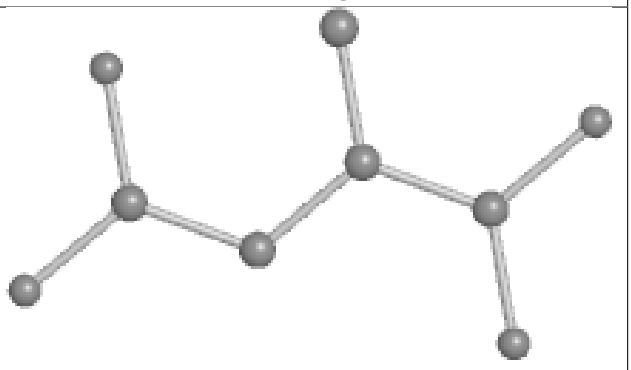
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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>2			OWAB(Å^2)	Q<0.9
1	A	540/585 (92%)	3.64	478 (88%)	0	0	12, 20, 34, 51	0
1	B	540/585 (92%)	3.76	480 (88%)	0	0	12, 20, 37, 49	0
1	C	528/585 (90%)	5.40	515 (97%)	0	0	20, 33, 48, 64	0
1	D	531/585 (90%)	5.01	501 (94%)	0	0	20, 34, 55, 69	0
All	All	2139/2340 (91%)	4.44	1974 (92%)	0	0	12, 28, 48, 69	0

The worst 5 of 1974 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	231	SER	21.5
1	C	183	LYS	15.4
1	C	545	PHE	14.2
1	D	88	ALA	14.1
1	D	38	VAL	14.1

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

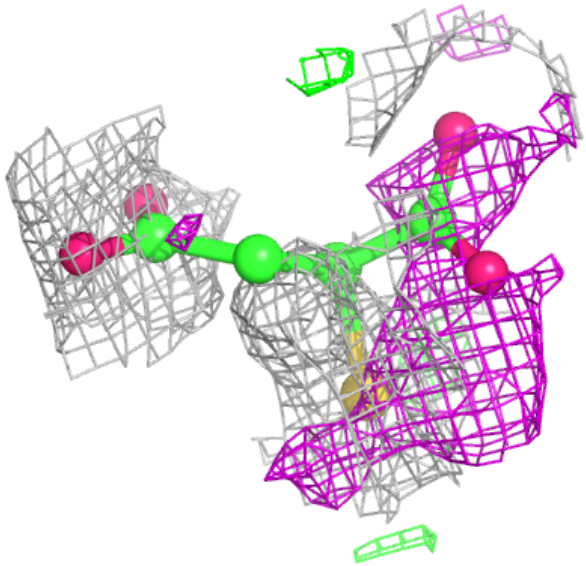
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

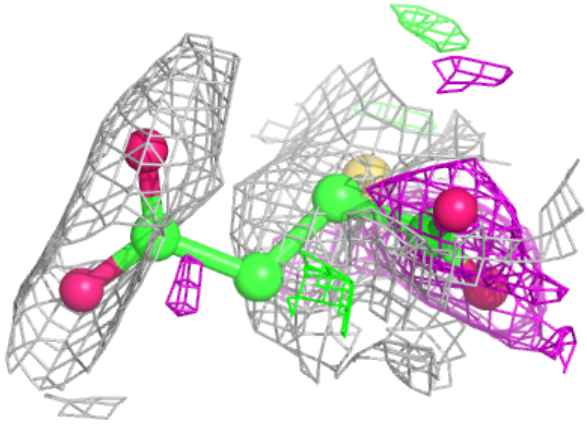
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	606	6/6	0.16	0.43	26,28,30,34	0
4	1PE	B	606	10/16	0.22	0.50	24,35,37,37	0
3	GOL	C	602	6/6	0.31	0.42	40,42,43,43	0
4	1PE	B	605	13/16	0.33	0.48	15,17,23,24	0
4	1PE	C	603	7/16	0.36	0.31	27,28,30,31	0
5	JYD	C	604	9/9	0.38	0.89	30,35,42,45	0
4	1PE	A	611	10/16	0.40	0.27	29,31,34,34	0
4	1PE	C	605	10/16	0.42	0.36	30,37,41,42	0
3	GOL	A	605	6/6	0.43	0.44	26,31,34,34	0
4	1PE	C	606	10/16	0.47	0.36	26,32,35,35	0
4	1PE	A	607	7/16	0.48	0.46	28,29,32,36	0
4	1PE	D	603	16/16	0.50	0.35	26,32,35,35	0
3	GOL	A	603	6/6	0.53	0.28	24,26,32,34	0
4	1PE	A	609	13/16	0.53	0.24	14,21,27,30	0
3	GOL	A	604	6/6	0.55	0.42	27,33,37,38	0
2	SF4	D	601	8/8	0.56	0.20	23,32,34,39	0
5	JYD	D	602	9/9	0.57	0.32	22,32,34,36	0
5	JYD	B	604[B]	9/9	0.60	0.34	9,10,12,14	9
4	1PE	A	610	10/16	0.60	0.27	10,29,36,39	0
5	JYD	B	604[A]	9/9	0.60	0.34	9,11,13,16	9
2	SF4	A	601	8/8	0.62	0.22	15,19,22,22	0
3	GOL	B	603	6/6	0.64	0.21	22,25,26,27	0
3	GOL	B	602	6/6	0.65	0.32	26,27,29,30	0
2	SF4	C	601	8/8	0.67	0.17	24,30,31,31	0
2	SF4	B	601	8/8	0.68	0.20	14,21,23,24	0
3	GOL	A	602	6/6	0.75	0.23	21,25,29,31	0
5	JYD	A	608[A]	9/9	0.81	0.30	17,17,18,21	9
5	JYD	A	608[B]	9/9	0.81	0.30	16,17,18,18	9

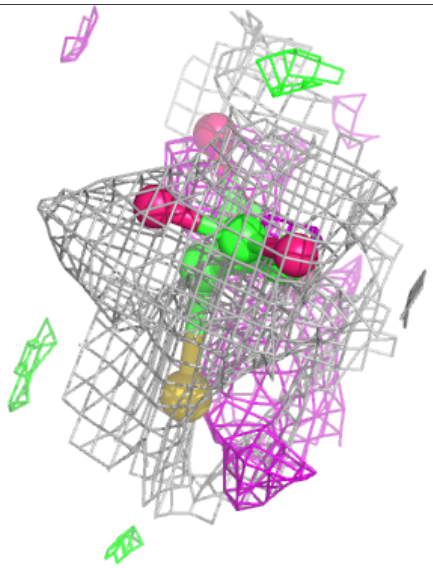
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JYD C 604:

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

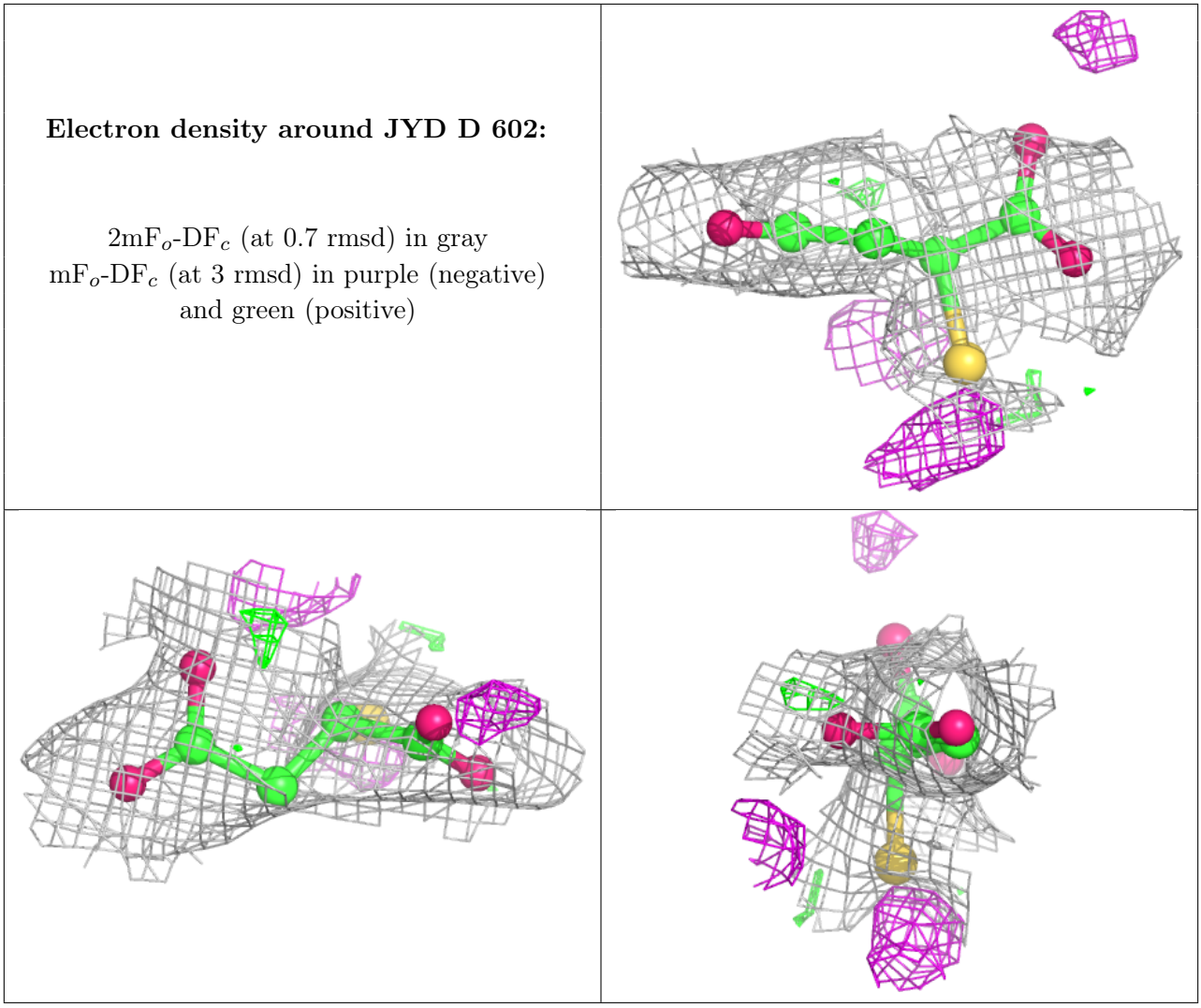






Electron density around JYD D 602:

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



Electron density around JYD B 604 (B):

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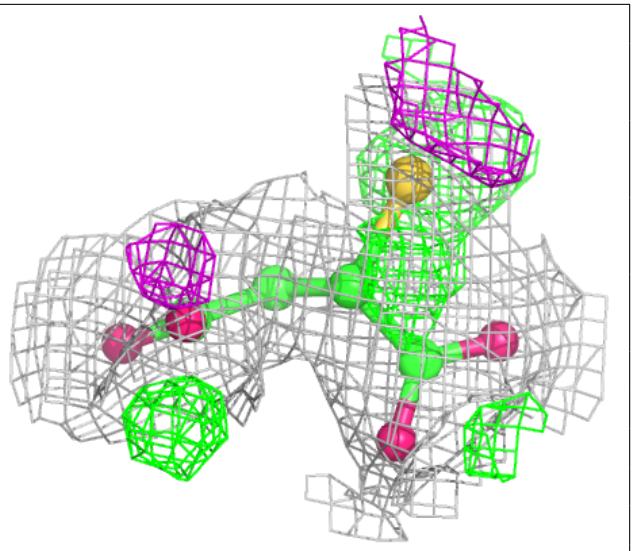
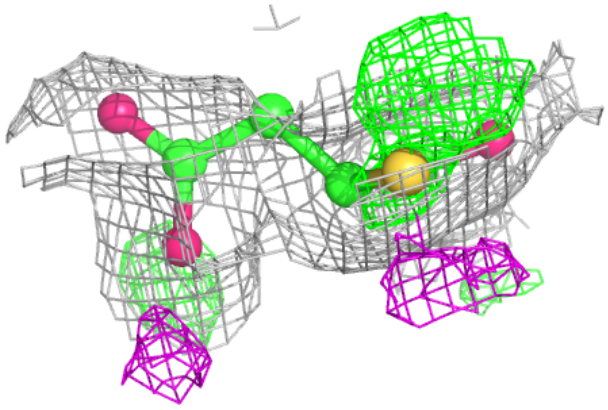
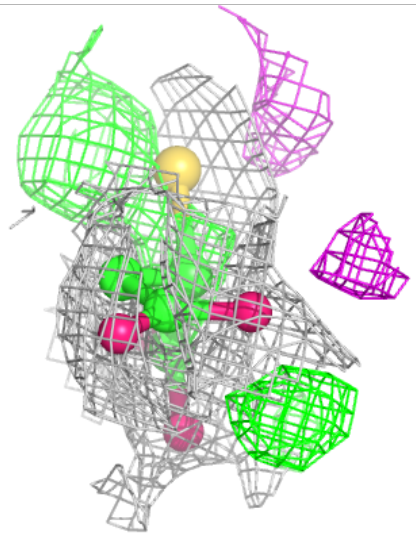
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

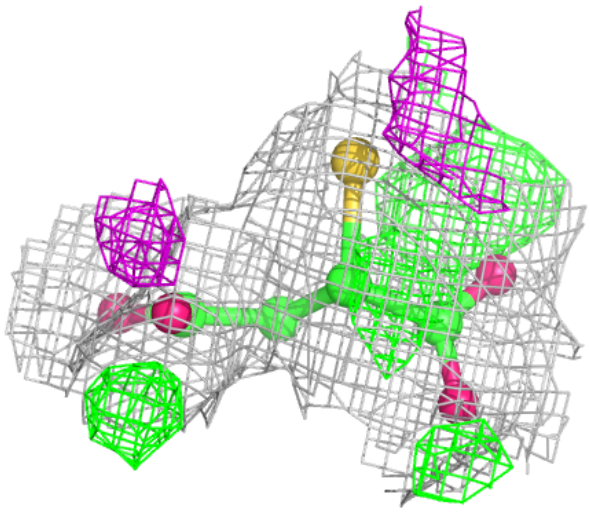


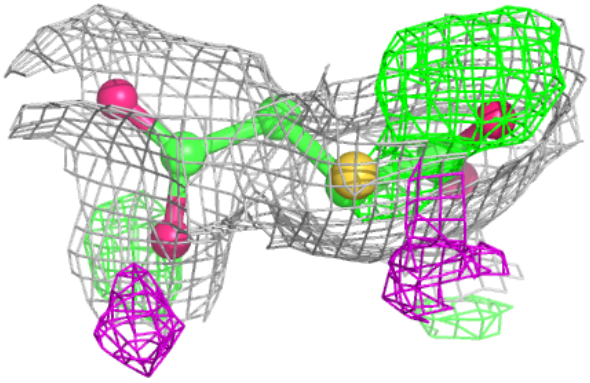


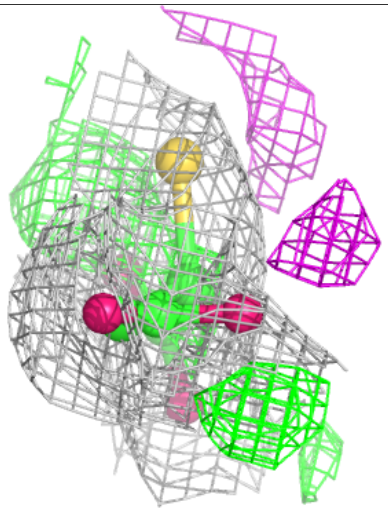


Electron density around JYD B 604 (A):

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

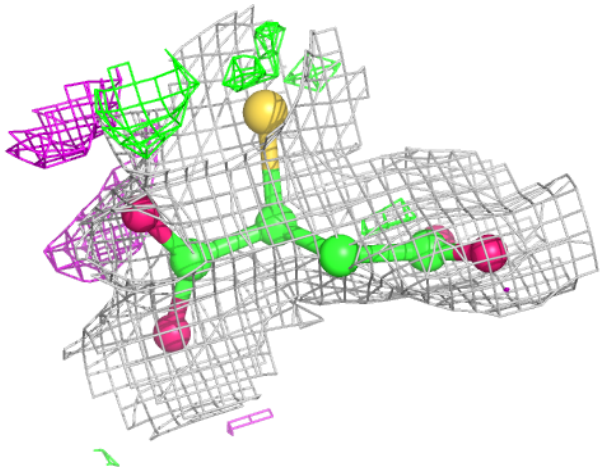


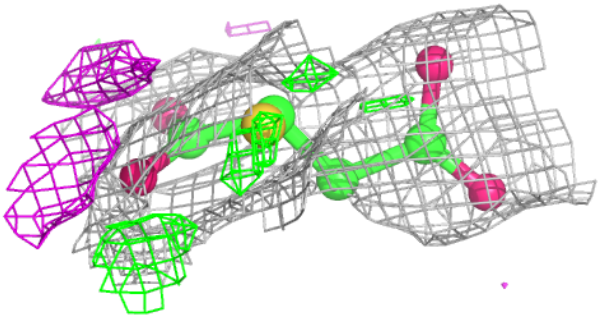


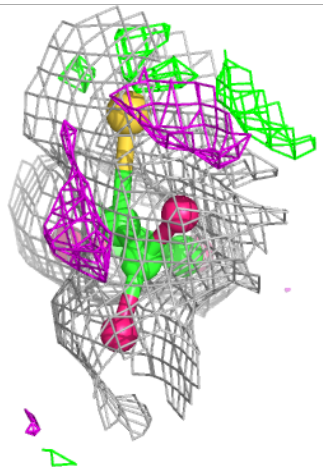


Electron density around JYD A 608 (A):

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







Electron density around JYD A 608 (B):

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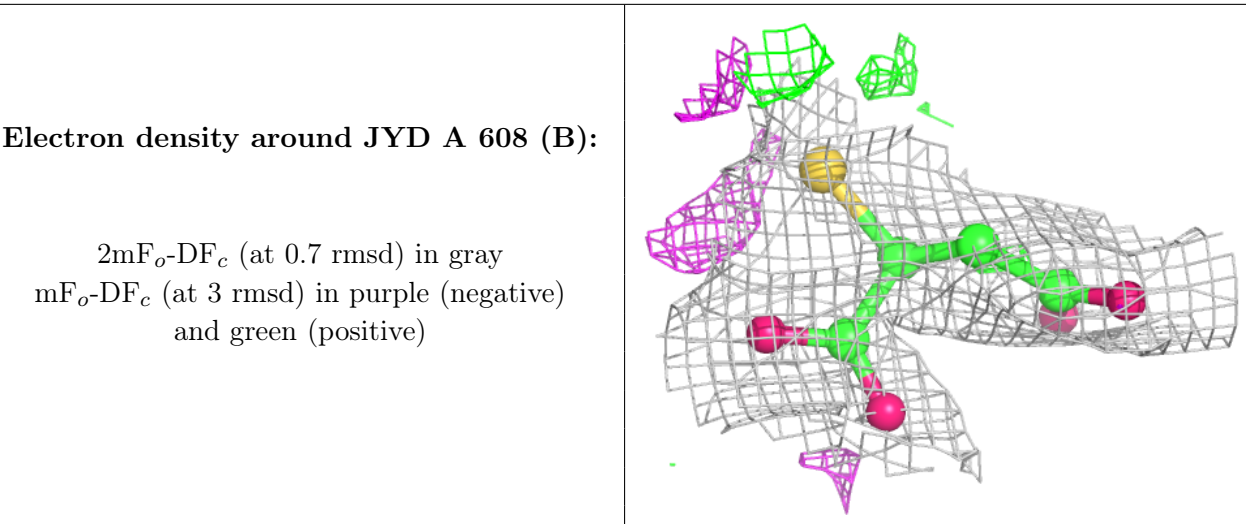
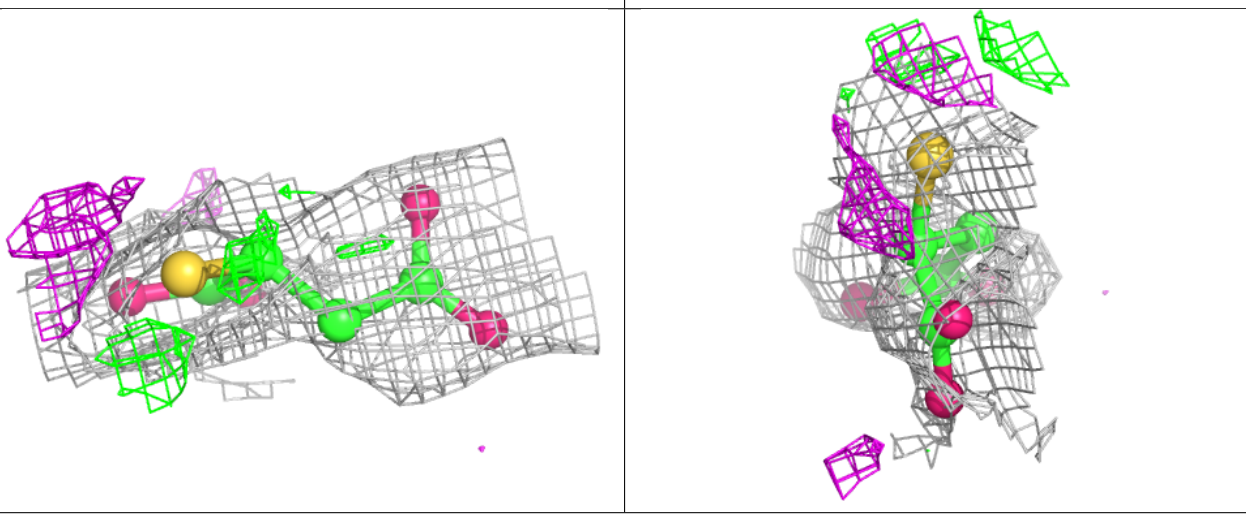
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers

There are no such residues in this entry.