



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 03:29 pm BST

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 ⓘ symbol.

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 : 2.11
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) : 2.11

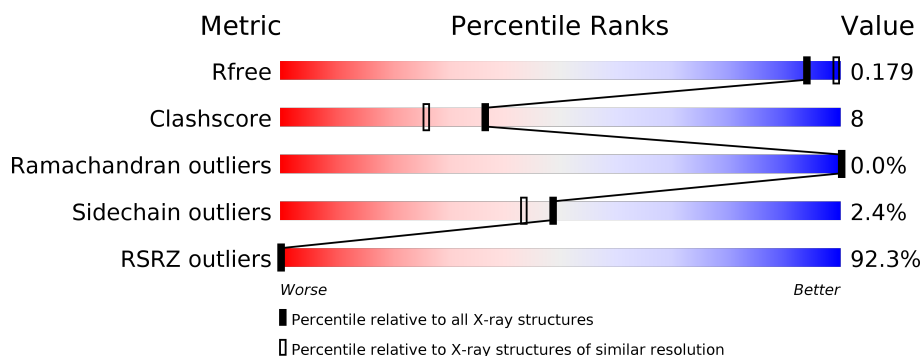
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	585	<div> <div>82%</div> <div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div>
1	B	585	<div> <div>82%</div> <div> <div>77%</div> <div>15%</div> <div>8%</div> </div> </div>
1	C	585	<div> <div>88%</div> <div> <div>69%</div> <div>20%</div> <div>10%</div> </div> </div>
1	D	585	<div> <div>86%</div> <div> <div>75%</div> <div>16%</div> <div>9%</div> </div> </div>

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 crite-

ria:

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

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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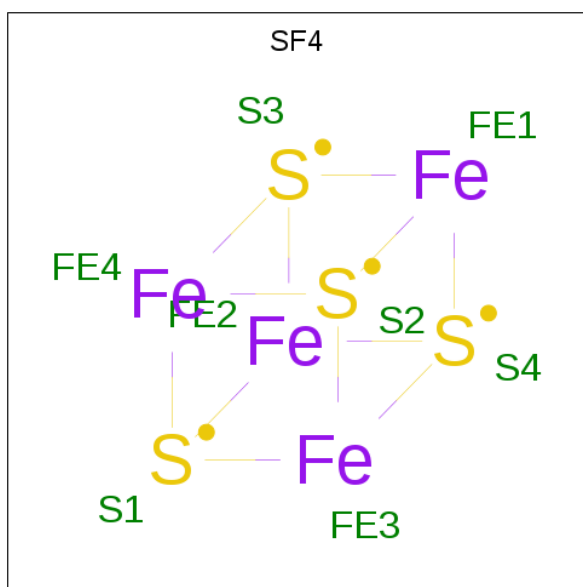
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B	-8	GLN	-	expression tag	UNP Q4QAU9
B	-7	GLN	-	expression tag	UNP Q4QAU9
B	-6	MET	-	expression tag	UNP Q4QAU9
B	-5	GLY	-	expression tag	UNP Q4QAU9
B	-4	ARG	-	expression tag	UNP Q4QAU9
B	-3	GLY	-	expression tag	UNP Q4QAU9
B	-2	SER	-	expression tag	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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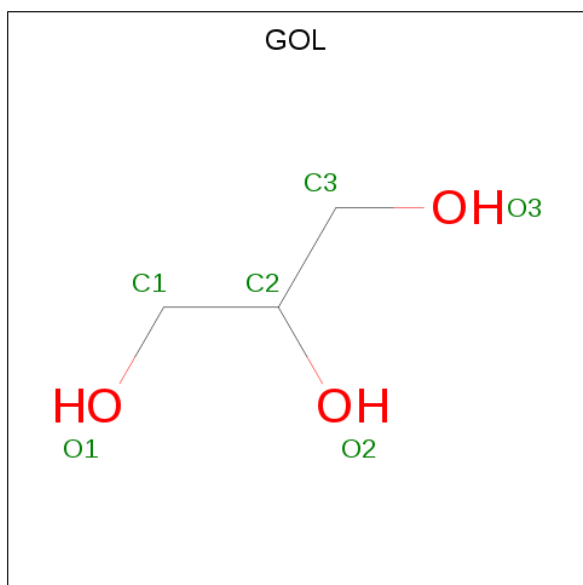
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP Q4QAU9
C	-1	GLU	-	expression tag	UNP Q4QAU9
C	0	PHE	-	expression tag	UNP Q4QAU9
D	-35	MET	-	initiating methionine	UNP Q4QAU9
D	-34	GLY	-	expression tag	UNP Q4QAU9
D	-33	SER	-	expression tag	UNP Q4QAU9
D	-32	SER	-	expression 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: Fe₄S₄).



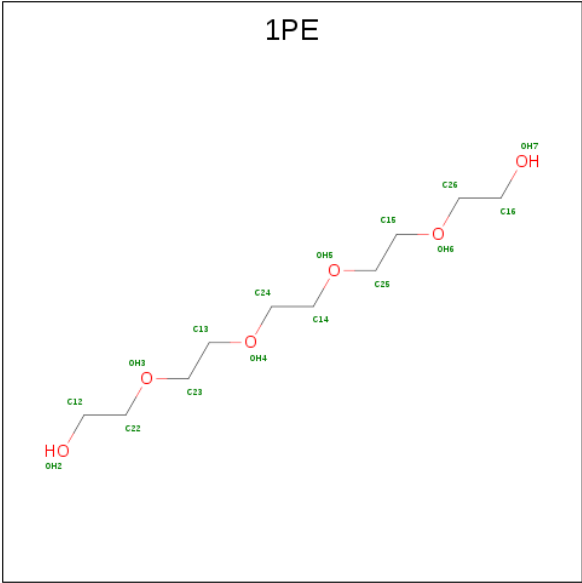
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

- 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	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



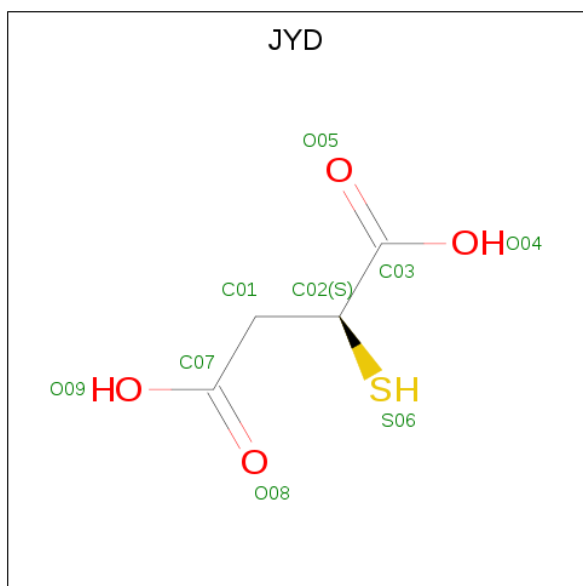
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		

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

- Molecule 5 is (2S)-2-sulfanylbutanedioic acid (three-letter code: JYD) (formula: C₄H₆O₄S) (labeled as "Ligand of Interest" by author).



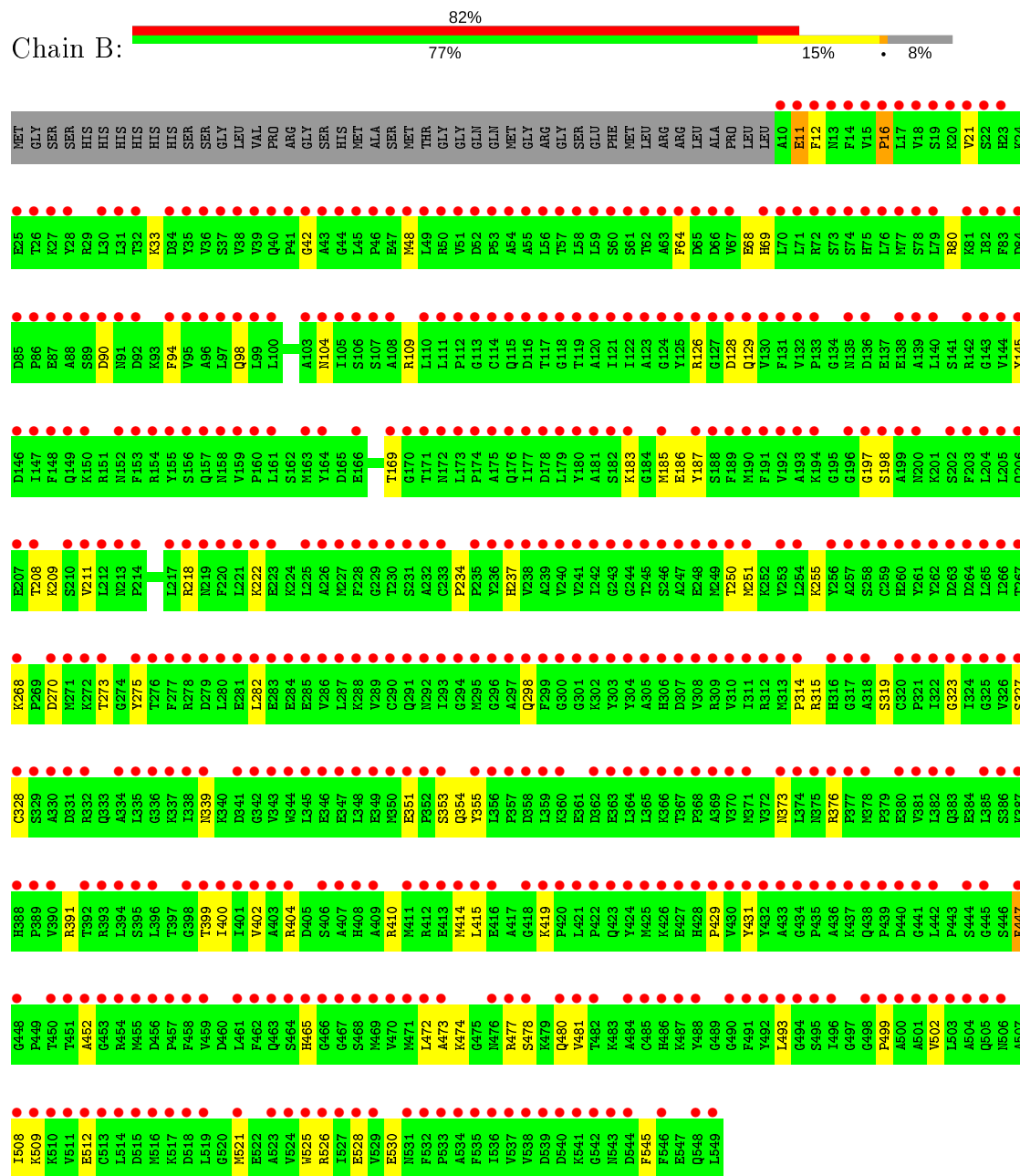
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	1
			18	8	8	2		
5	B	1	Total	C	O	S	0	1
			18	8	8	2		
5	C	1	Total	C	O	S	0	0
			9	4	4	1		
5	D	1	Total	C	O	S	0	0
			9	4	4	1		

- Molecule 6 is water.

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

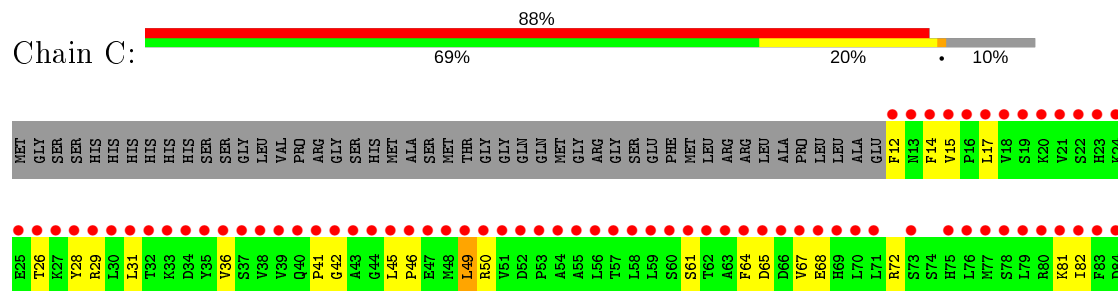
- Molecule 1: fumarate hydratase

Chain B:



- Molecule 1: fumarate hydratase

Chain C:



Q505	N506	A507	I508	K509	K510	V511	E512	G513	L514	D515	M516	K517	D518	L519	G520	M521	E522	A523	V524	M525	R526	I527	E528	V529	E530	N531	F532	P533	A534	F535	I536	V537	D538	D539	D540	K541	G542	N543	D544	F545	F546	E547	Q548	LEU															
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	I496	G497	G498	P499	A500	A501	V502	L503	A504
L385	S386	K387	E388	P389	V390	R391	T392	R393	L394	S395	L396	T397	G398	T399	K400	L401	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
G325	V326	S327	C328	S329	A330	D331	R332	Q333	A334	L335	G336	K337	I338	R339	K340	D341	G342	V343	V344	L345	E346	E347	L348	F349	K350	E351	P352	S353	Q354	Y355	L356	F357	D358	L359	K360	GLU	ASP	GLU	LEU	LEU	LYS	T367	P368	A369	V370	K371	V372	V373	L374	R375	R376	F377	K378	P379	F380	V381	L382	Q383	E384
L265	I266	T267	R268	F269	D270	K271	K272	T273	G274	V275	T276	F277	R278	D279	L280	E281	L282	E283	E284	E285	V286	L287	K288	V289	C290	Q291	N292	I293	Q294	K295	G296	A297	Q298	F299	G300	G301	K302	Y303	Y304	A305	H306	D307	V308	R309	V310	I311	R312	K313	P314	R315	R316	G317	A318	S319	C320	P321	I322	G323	I324

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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 [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	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 ⓘ

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	17	LEU
1	C	268	LYS
1	D	447	PHE
1	C	187	TYR
1	C	218[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	SF4	A	601	1,5	0,12,12	0.00	-	-		
2	SF4	D	601	1,5	0,12,12	0.00	-	-		
4	1PE	B	605	-	12,12,15	0.55	0	11,11,14	0.67	0
4	1PE	C	605	-	9,9,15	0.27	0	8,8,14	0.50	0
3	GOL	C	602	-	5,5,5	0.90	0	5,5,5	1.05	0
4	1PE	C	603	-	6,6,15	0.50	0	5,5,14	0.37	0
3	GOL	A	604	-	5,5,5	1.16	1 (20%)	5,5,5	1.10	0
4	1PE	C	606	-	9,9,15	0.26	0	8,8,14	0.50	0
3	GOL	B	603	-	5,5,5	1.19	1 (20%)	5,5,5	1.09	0
4	1PE	D	603	-	15,15,15	0.55	0	14,14,14	0.39	0
3	GOL	A	606	-	5,5,5	1.15	1 (20%)	5,5,5	1.00	0
2	SF4	B	601	1,5	0,12,12	0.00	-	-		
4	1PE	A	611	-	9,9,15	0.28	0	8,8,14	0.39	0
5	JYD	B	604[A]	2	1,8,8	0.28	0	0,10,10	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	JYD	B	604[B]	2	1,8,8	0.12	0	0,10,10	0.00	-
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
5	JYD	A	608[B]	2	1,8,8	0.03	0	0,10,10	0.00	-
3	GOL	A	603	-	5,5,5	1.30	1 (20%)	5,5,5	0.93	0
3	GOL	A	605	-	5,5,5	1.30	1 (20%)	5,5,5	0.80	0
5	JYD	A	608[A]	2	1,8,8	0.31	0	0,10,10	0.00	-
3	GOL	B	602	-	5,5,5	0.84	0	5,5,5	1.56	1 (20%)
4	1PE	A	607	-	6,6,15	0.50	0	5,5,14	0.38	0
5	JYD	C	604	2	1,8,8	0.07	0	0,10,10	0.00	-
5	JYD	D	602	2	1,8,8	0.17	0	0,10,10	0.00	-
3	GOL	A	602	-	5,5,5	1.72	1 (20%)	5,5,5	1.08	1 (20%)
4	1PE	A	610	-	9,9,15	0.36	0	8,8,14	0.35	0
2	SF4	C	601	1,5	0,12,12	0.00	-	-	-	-

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	SF4	A	601	1,5	-	-	0/6/5/5
2	SF4	D	601	1,5	-	-	0/6/5/5
4	1PE	B	605	-	-	3/10/10/13	-
4	1PE	C	605	-	-	4/7/7/13	-
3	GOL	C	602	-	-	2/4/4/4	-
4	1PE	C	603	-	-	4/4/4/13	-
3	GOL	A	604	-	-	4/4/4/4	-
4	1PE	C	606	-	-	3/7/7/13	-
3	GOL	B	603	-	-	0/4/4/4	-
4	1PE	D	603	-	-	11/13/13/13	-
3	GOL	A	606	-	-	2/4/4/4	-
2	SF4	B	601	1,5	-	-	0/6/5/5
4	1PE	A	611	-	-	5/7/7/13	-
5	JYD	B	604[A]	2	-	1/2/8/8	-
5	JYD	B	604[B]	2	-	2/2/8/8	-
4	1PE	B	606	-	-	4/7/7/13	-
4	1PE	A	609	-	-	7/10/10/13	-
5	JYD	A	608[B]	2	-	1/2/8/8	-

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

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

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	GOL	C3-C2-C1	-2.63	101.50	111.70
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	C	602	GOL	O1-C1-C2-C3
3	A	604	GOL	O1-C1-C2-C3
3	A	606	GOL	C1-C2-C3-O3
5	B	604[A]	JYD	C07-C01-C02-S06
5	B	604[B]	JYD	C07-C01-C02-C03

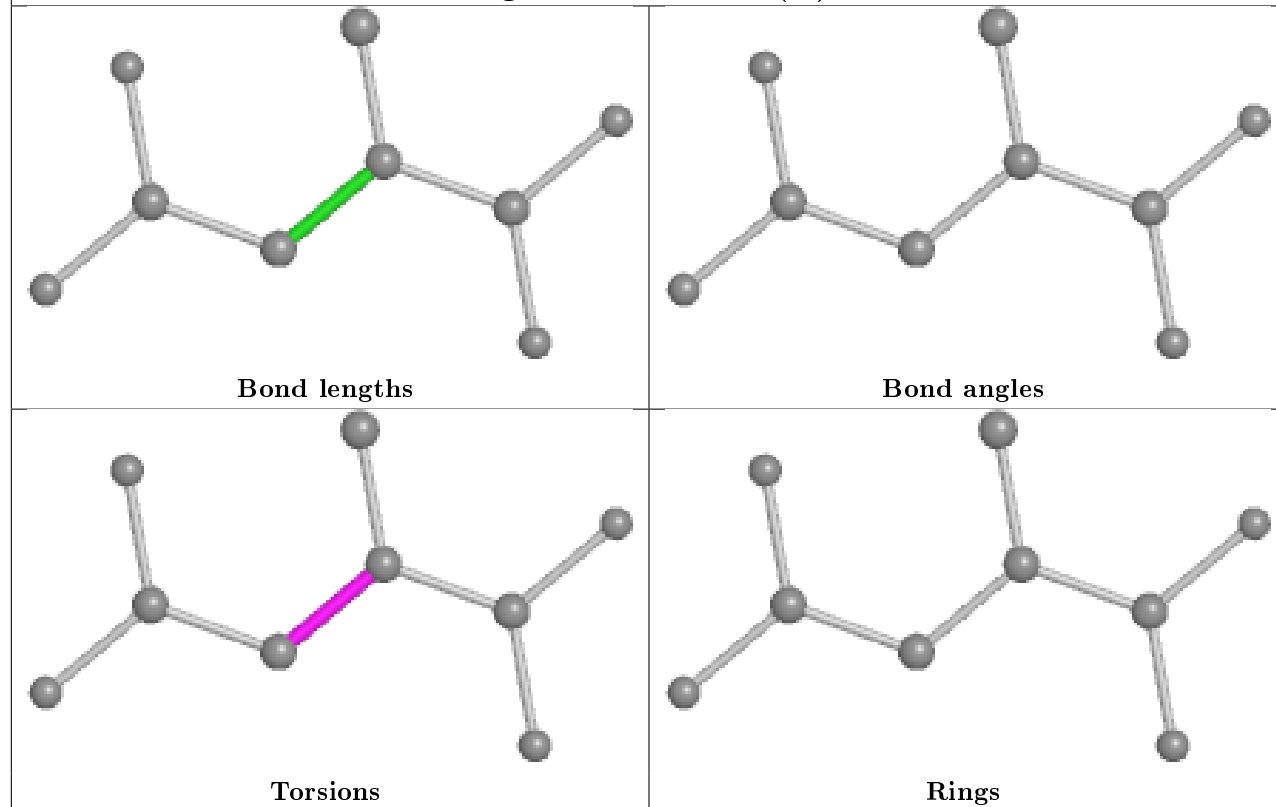
There are no ring outliers.

20 monomers are involved in 31 short contacts:

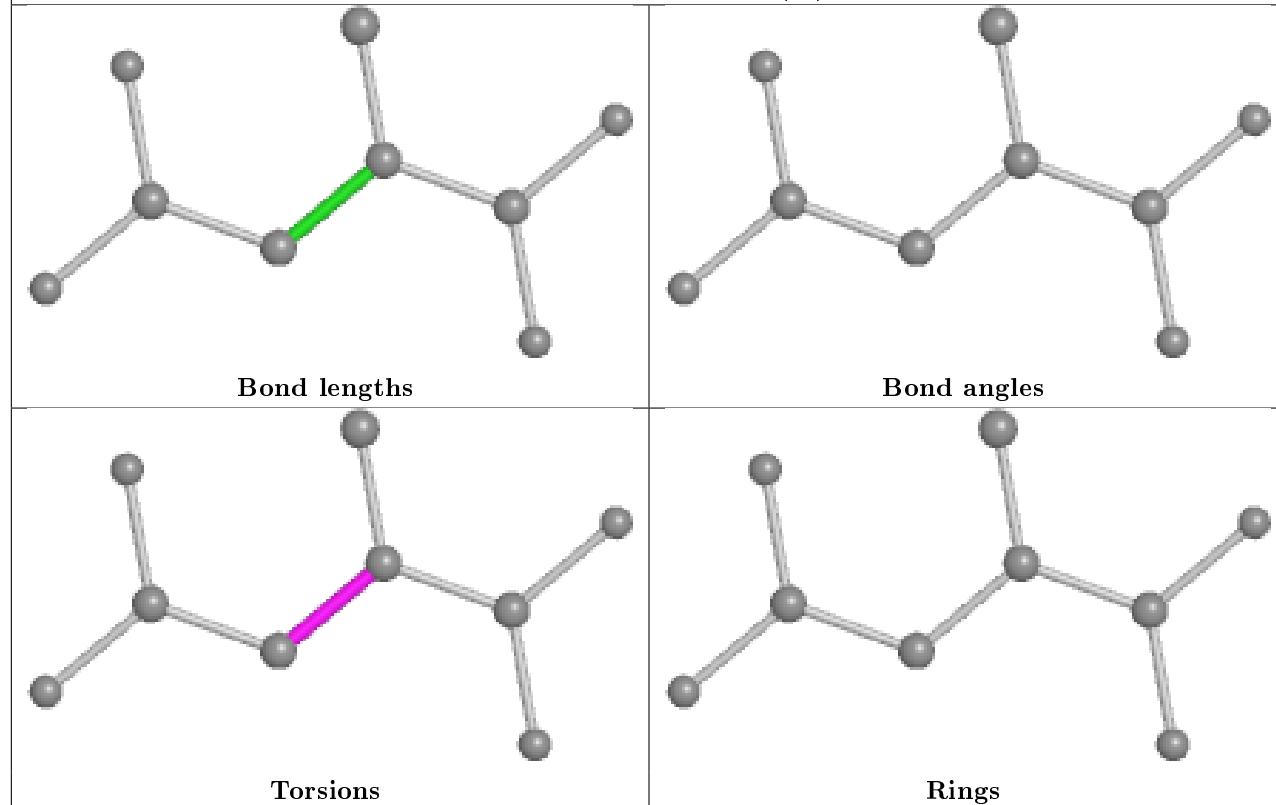
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	605	1PE	2	0
4	C	605	1PE	2	0
3	C	602	GOL	3	0
4	C	603	1PE	1	0
3	A	604	GOL	1	0
4	C	606	1PE	1	0
4	D	603	1PE	4	0
4	A	611	1PE	1	0
5	B	604[A]	JYD	1	0
5	B	604[B]	JYD	1	0
4	B	606	1PE	1	0
4	A	609	1PE	2	0
5	A	608[B]	JYD	3	0
3	A	603	GOL	1	0
5	A	608[A]	JYD	1	0
3	B	602	GOL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

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

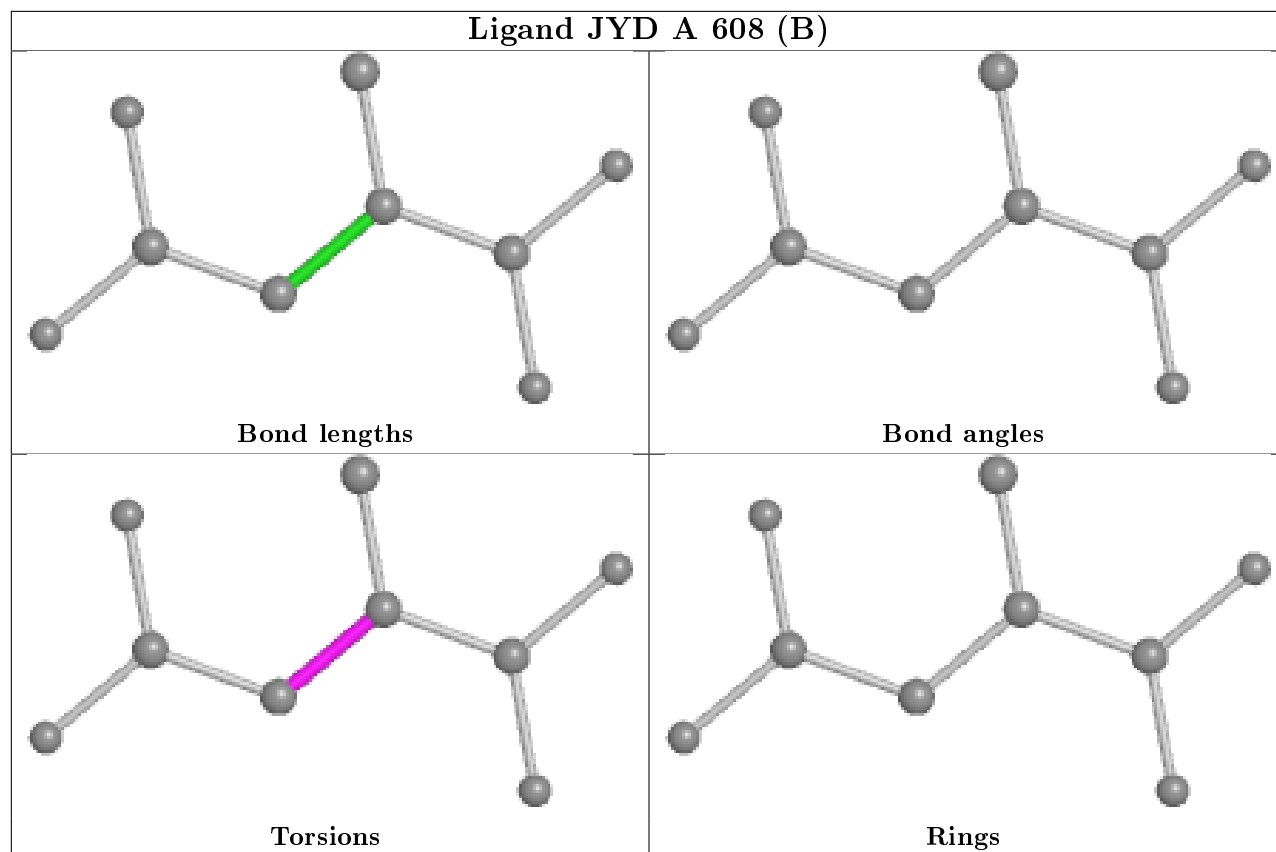
Ligand JYD B 604 (A)



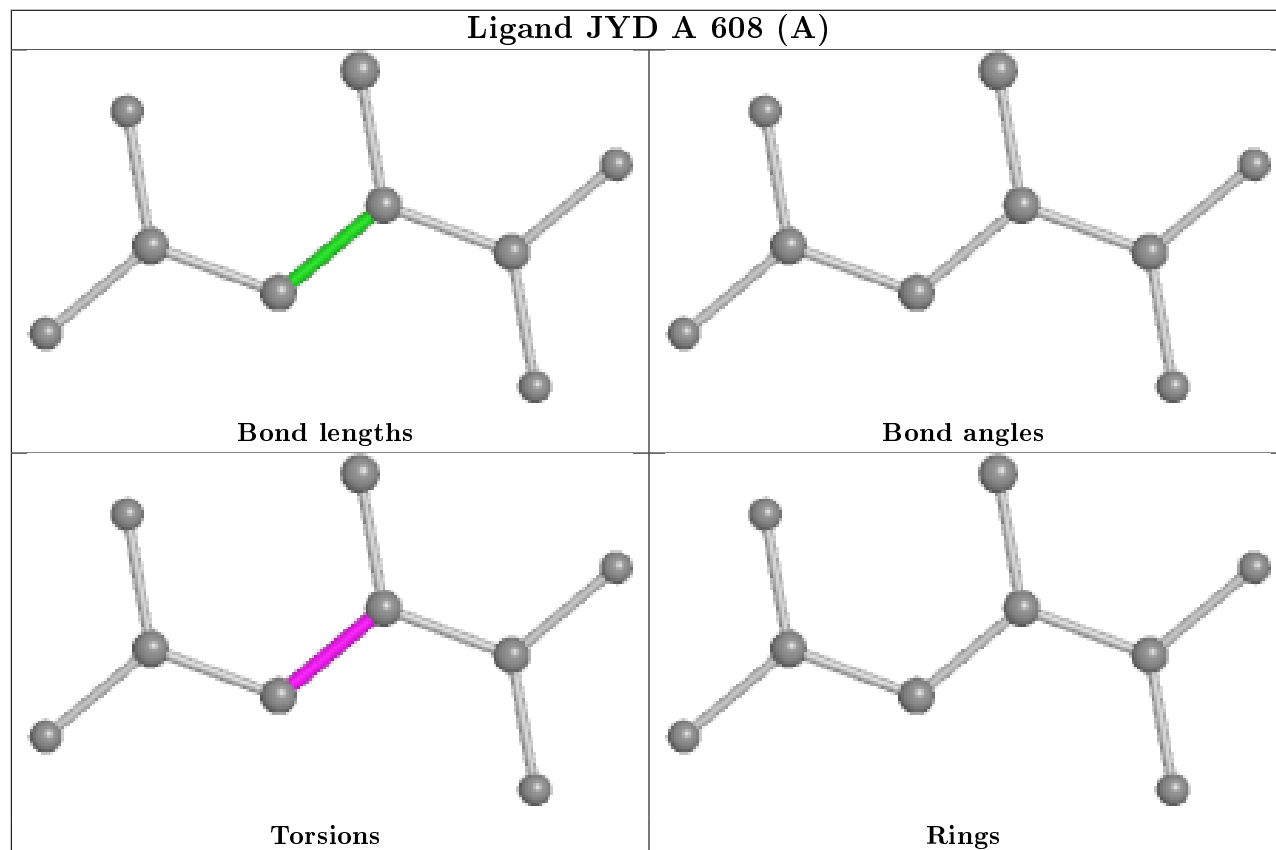
Ligand JYD B 604 (B)



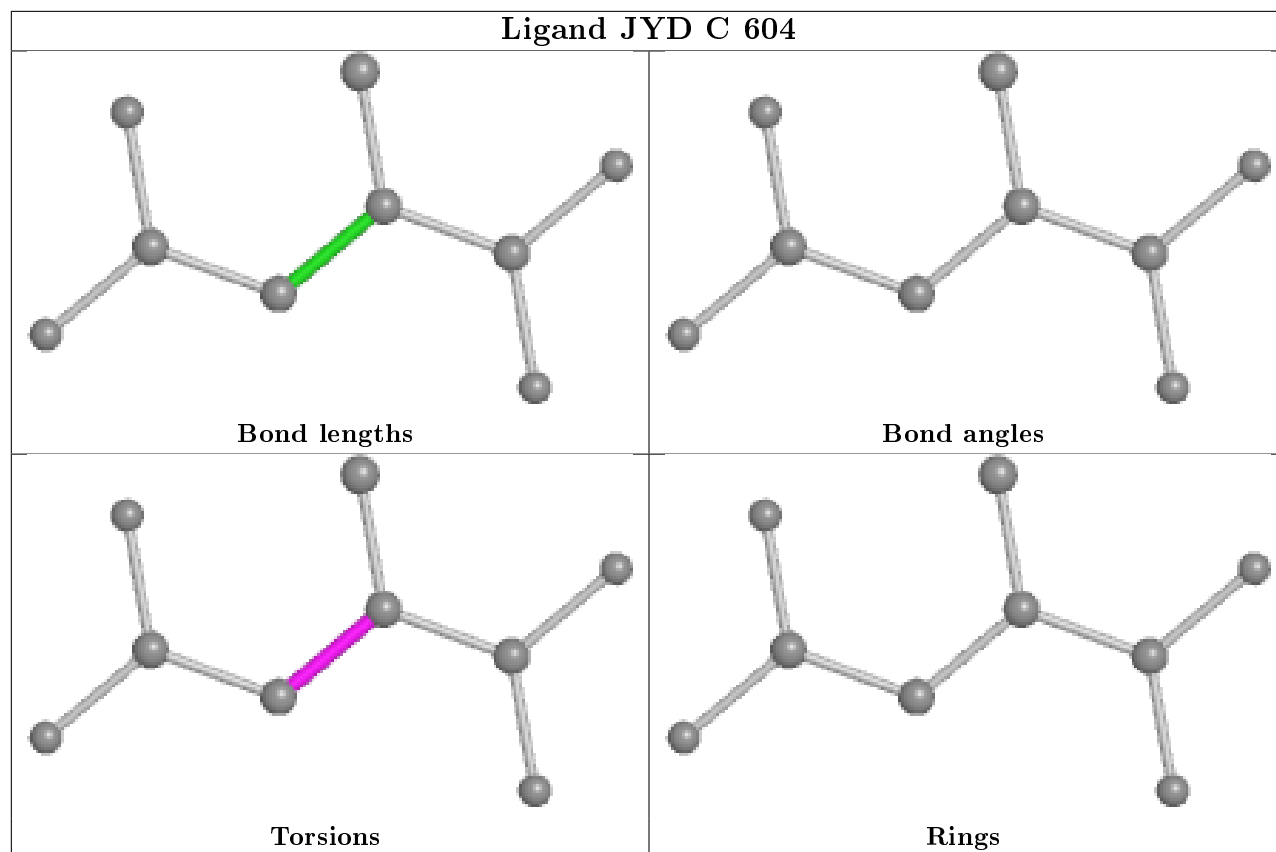
Ligand JYD A 608 (B)



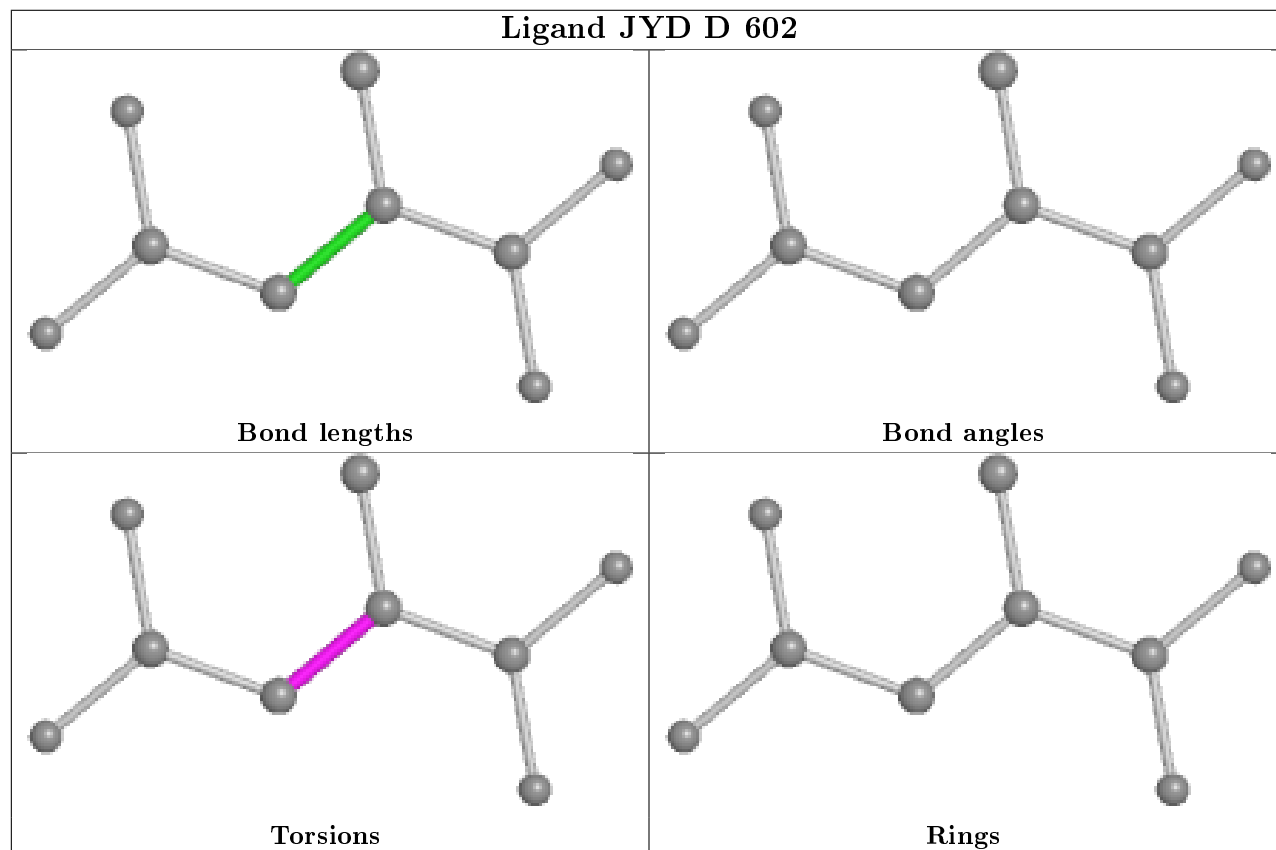
Ligand JYD A 608 (A)



Ligand JYD C 604



Ligand JYD D 602



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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 [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

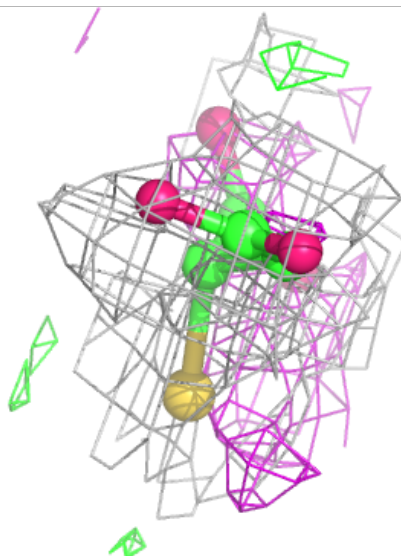
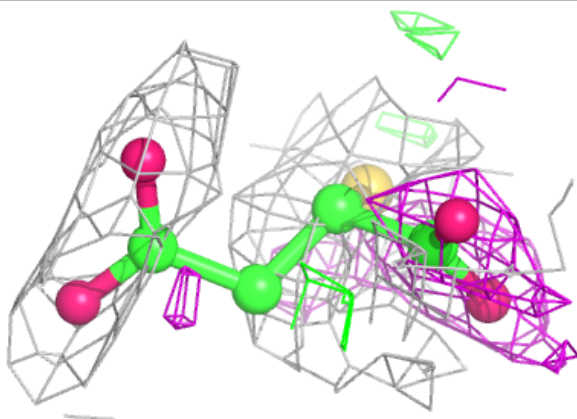
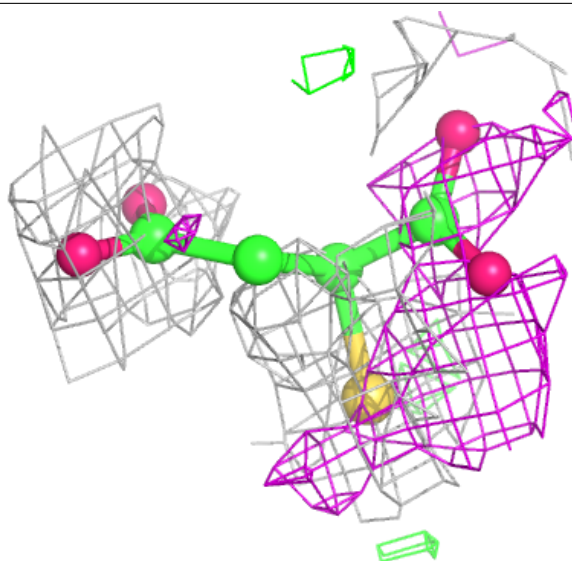
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^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
5	JYD	B	604[A]	9/9	0.60	0.34	9,11,13,16	9
4	1PE	A	610	10/16	0.60	0.27	10,29,36,39	0
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.

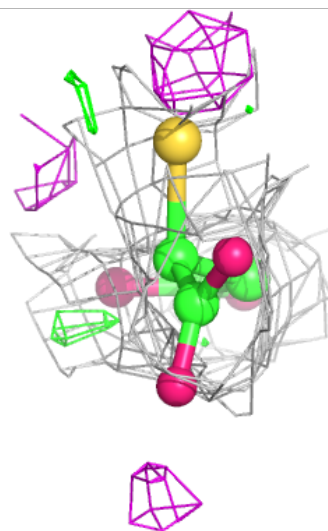
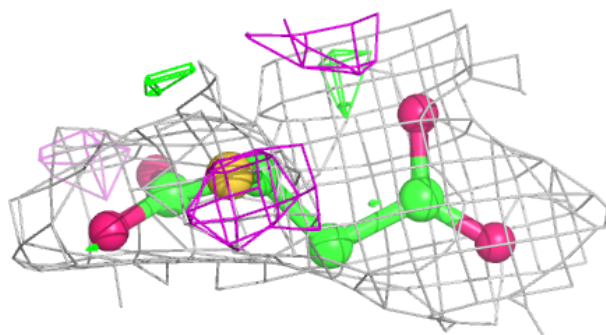
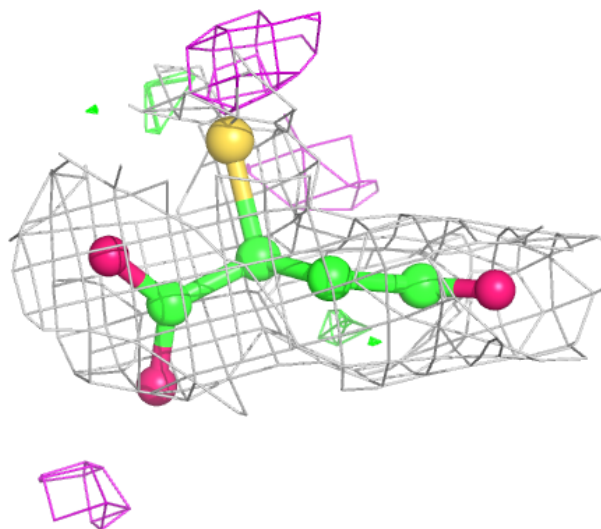
Electron density around JYD C 604:

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



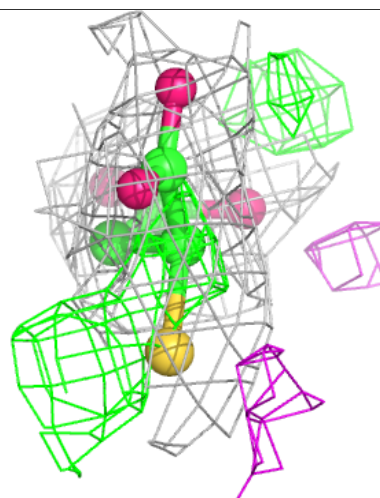
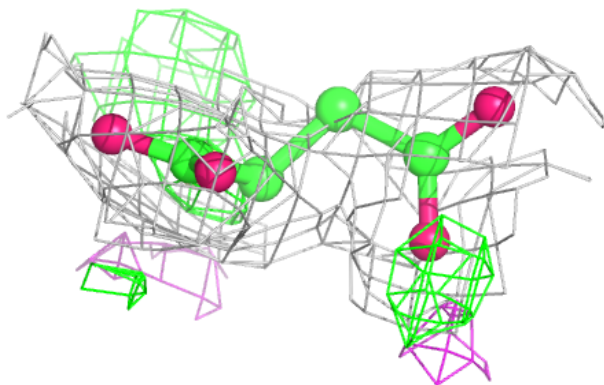
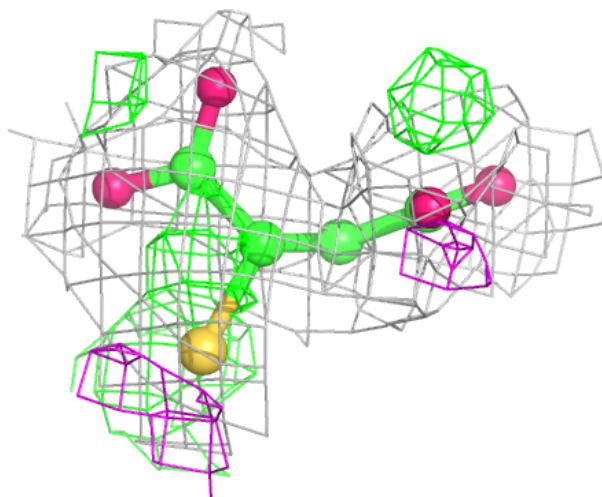
Electron density around JYD D 602:

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



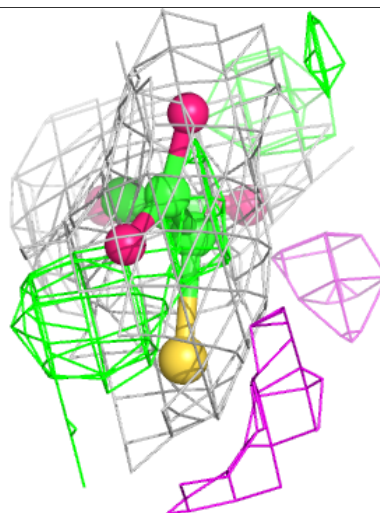
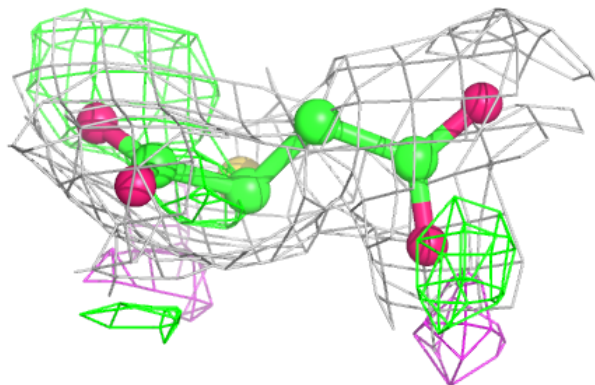
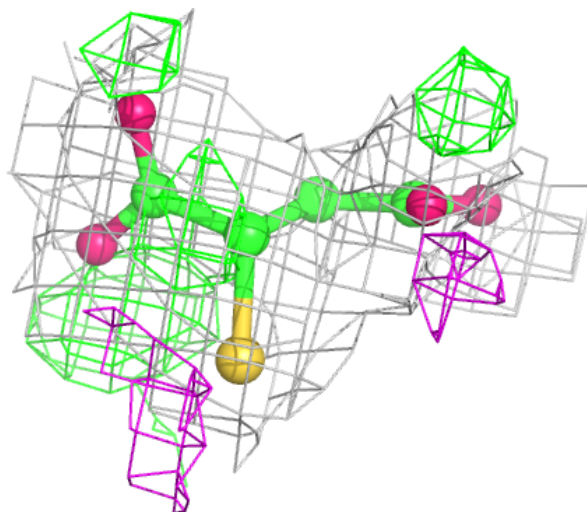
Electron density around JYD B 604 (B):

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



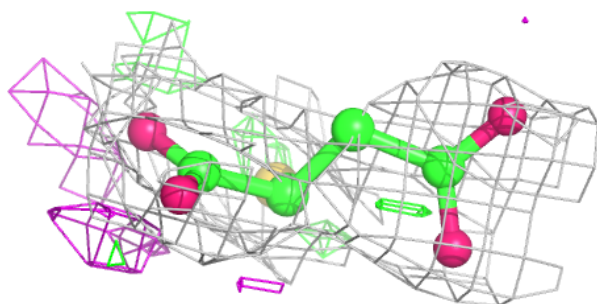
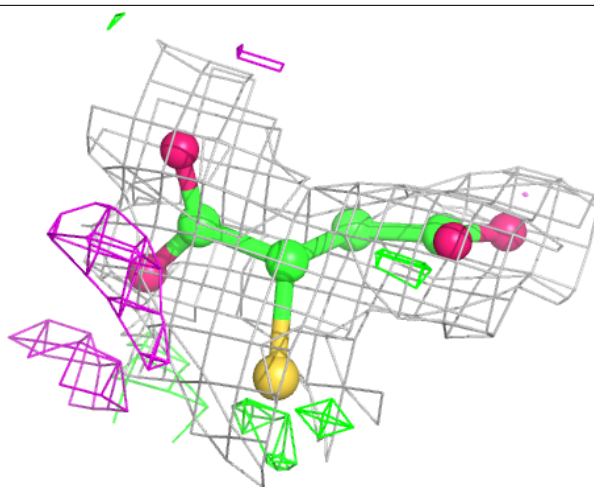
Electron density around JYD B 604 (A):

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



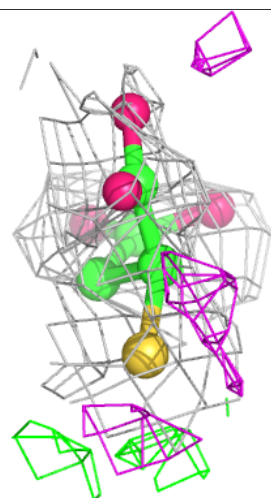
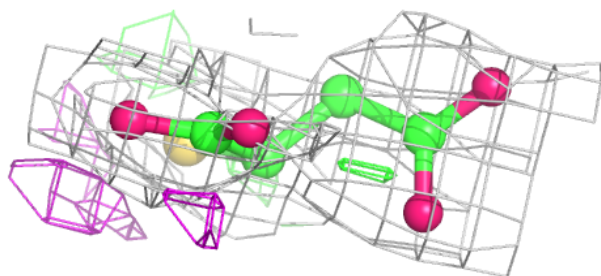
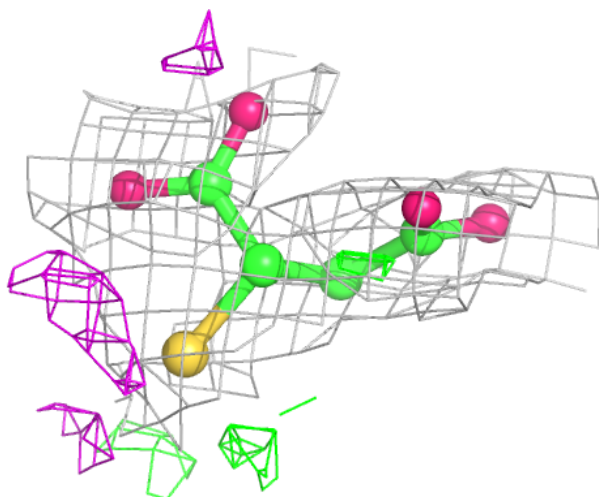
Electron density around JYD A 608 (A):

$2mF_o-DF_c$ (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):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.