



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:08 PM UTC

PDB ID : 6MSO / pdb_00006mso
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

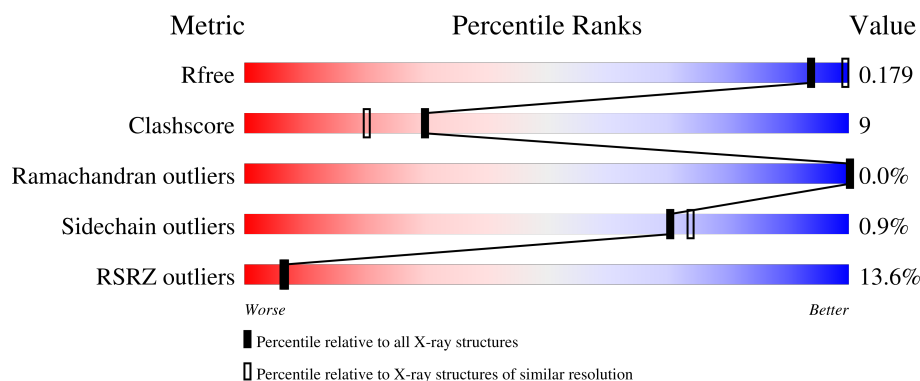
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (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 $\leq 5\%$. 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	
1	B	585	
1	C	585	
1	D	585	

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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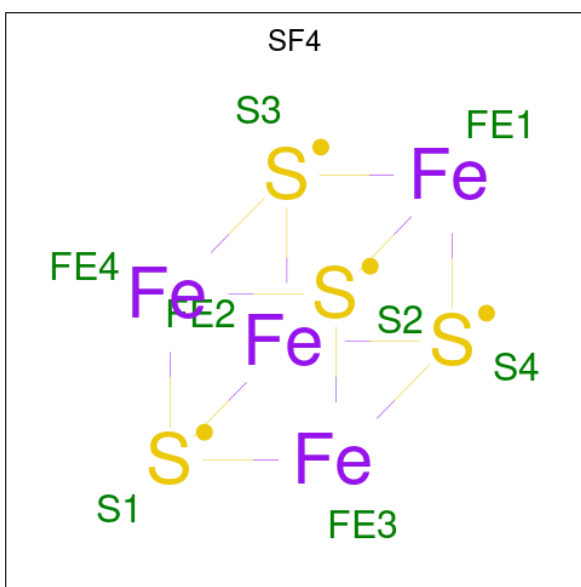
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLN	-	expression tag	UNP Q4QAU9
B	-7	GLN	-	expression tag	UNP Q4QAU9
B	-6	MET	-	expression tag	UNP Q4QAU9
B	-5	GLY	-	expression tag	UNP Q4QAU9
B	-4	ARG	-	expression tag	UNP Q4QAU9
B	-3	GLY	-	expression tag	UNP Q4QAU9
B	-2	SER	-	expression tag	UNP Q4QAU9
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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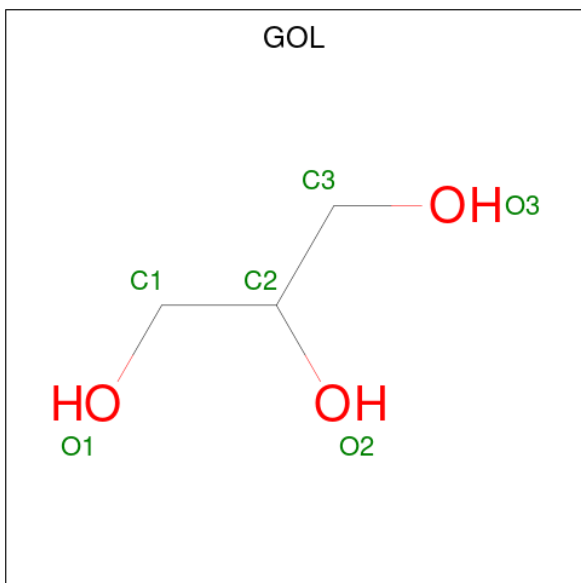
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP Q4QAU9
C	-1	GLU	-	expression tag	UNP Q4QAU9
C	0	PHE	-	expression tag	UNP Q4QAU9
D	-35	MET	-	initiating methionine	UNP Q4QAU9
D	-34	GLY	-	expression tag	UNP Q4QAU9
D	-33	SER	-	expression tag	UNP Q4QAU9
D	-32	SER	-	expression 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 (CCD ID: SF4) (formula: Fe₄S₄).



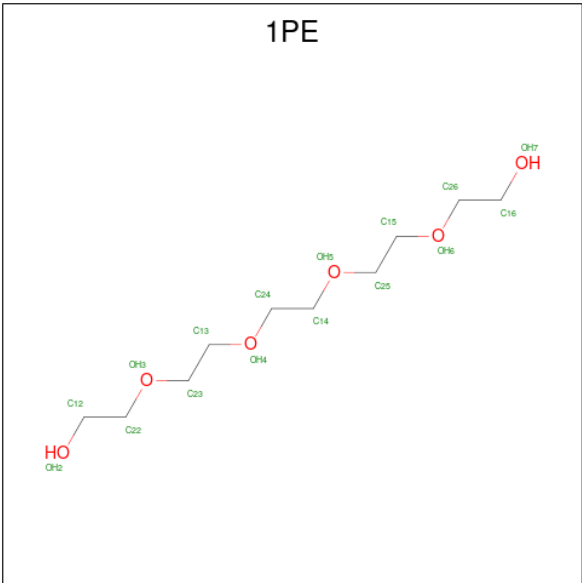
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is GLYCEROL (CCD ID: 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 (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



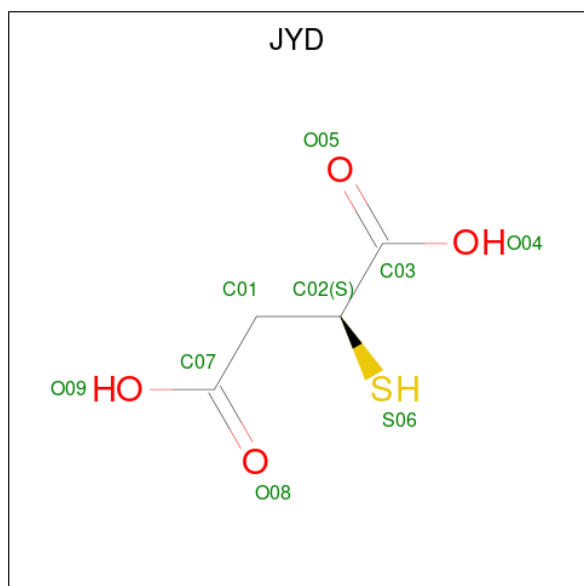
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		

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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 (CCD ID: 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	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		

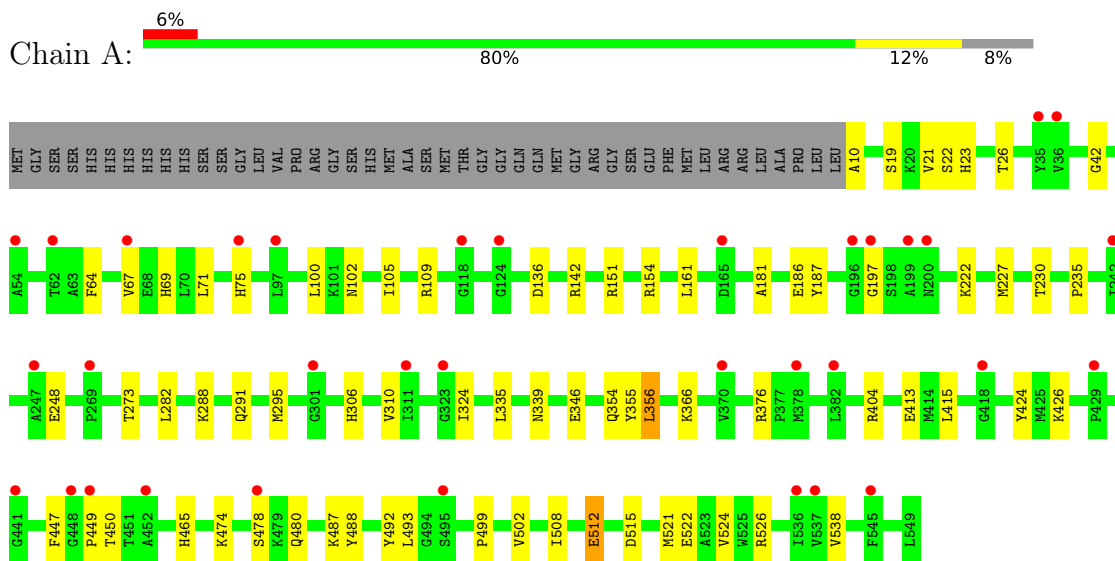
- Molecule 6 is water.

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

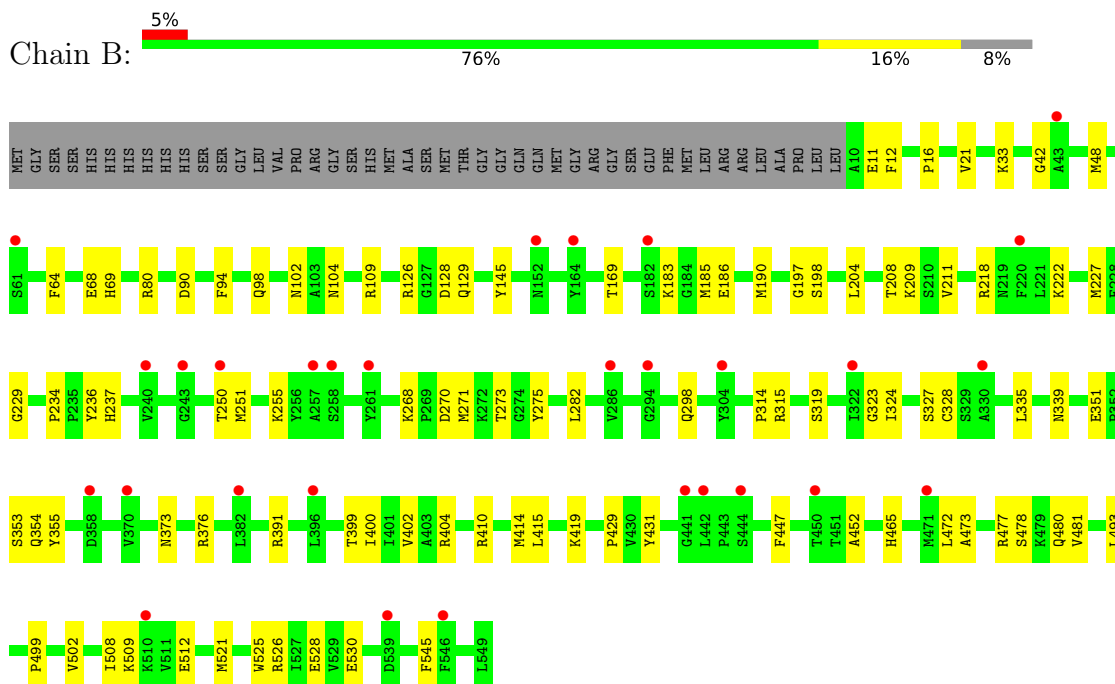
3 Residue-property plots

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: fumarate hydratase

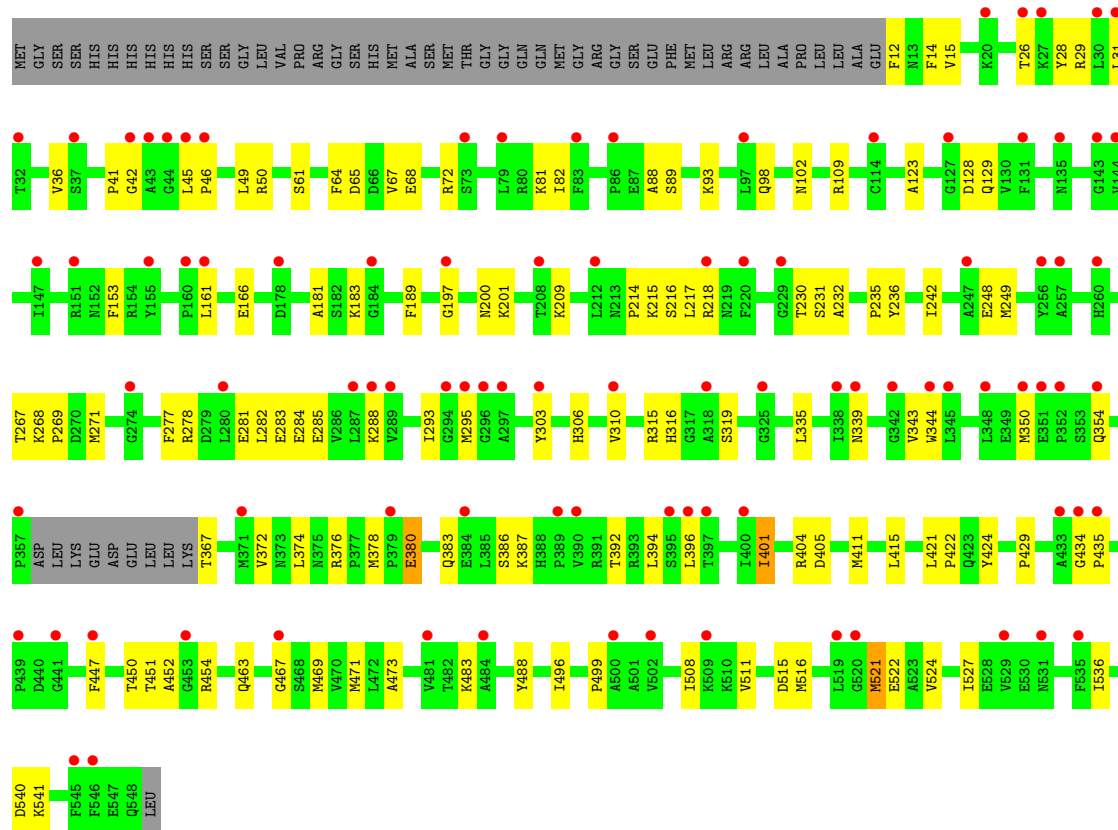


- Molecule 1: fumarate hydratase



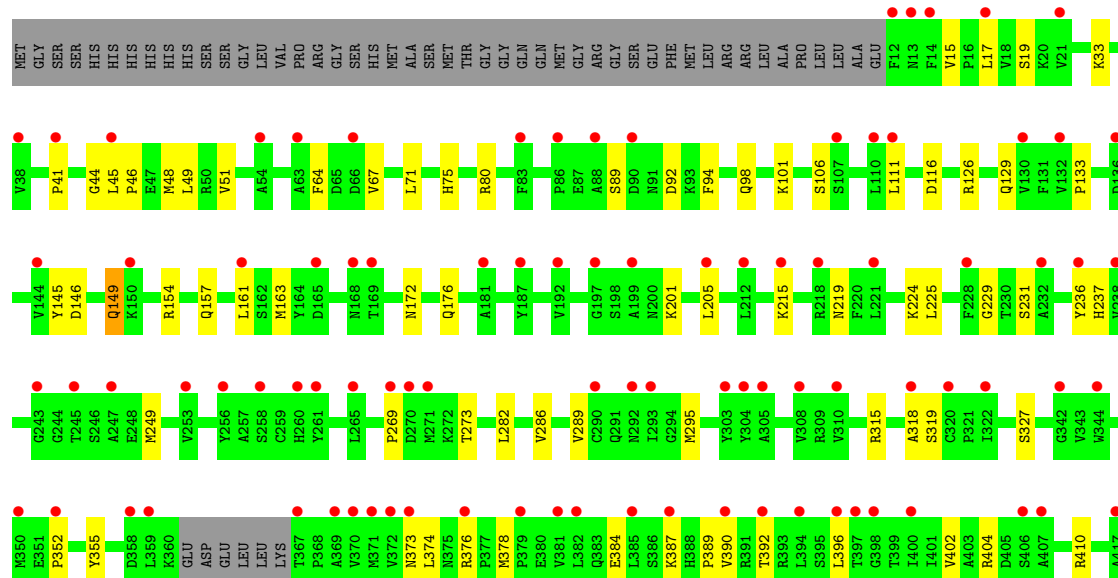
• Molecule 1: fumarate hydratase

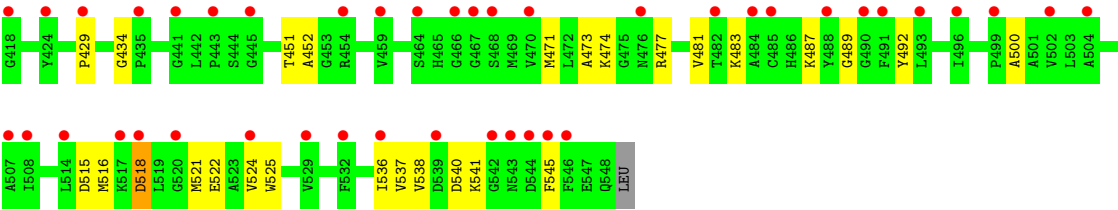
Chain C: 



• Molecule 1: fumarate hydratase

Chain D: 





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 (4.96%)	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 , 51.5	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	0.91	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: JYD, SF4, GOL, 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	0.39	0/4259	0.57	0/5761
1	B	0.39	0/4264	0.58	0/5768
1	C	0.34	0/4144	0.58	0/5609
1	D	0.33	0/4128	0.56	0/5595
All	All	0.36	0/16795	0.57	0/22733

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	4169	0	4113	51	0
1	B	4174	0	4120	70	0
1	C	4055	0	3975	93	0
1	D	4039	0	3915	79	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
3	A	30	0	37	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	0
6	B	282	0	0	8	0
6	C	167	0	0	5	0
6	D	169	0	0	6	0
All	All	17547	0	16317	281	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 9.

All (281) 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:C:242:ILE:HG13	1:D:163:MET:HE1	1.48	0.93
1:B:391:ARG:NH2	6:B:701:HOH:O	2.00	0.91
1:A:42:GLY:H	1:B:42:GLY:H	1.23	0.84
1:D:434:GLY:HA3	1:D:521:MET:CE	2.07	0.83
1:C:41:PRO:HB2	1:D:41:PRO:HB2	1.61	0.83
1:C:521:MET:HE2	1:C:522:GLU:HG2	1.62	0.82
1:D:434:GLY:HA3	1:D:521:MET:HE3	1.62	0.81
1:D:33:LYS:HD2	4:D:603:1PE:H222	1.64	0.79
1:D:410:ARG:NH1	1:D:518[A]:ASP:OD2	2.16	0.79
1:C:267:THR:O	1:C:268:LYS:CD	2.31	0.77
1:B:48:MET:HE2	6:B:910:HOH:O	1.85	0.75
1:A:230:THR:HG23	1:A:295:MET:HE2	1.67	0.74
1:B:509:LYS:HG3	1:B:530:GLU:HG3	1.67	0.74
1:C:166:GLU:OE1	1:D:315:ARG:NE	2.21	0.74
4:D:603:1PE:H161	4:D:603:1PE:H241	1.69	0.73
1:D:477:ARG:HD3	1:D:481:VAL:HG11	1.70	0.73
1:D:410:ARG:HB3	1:D:516:MET:HE1	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:GOL:O3	3:B:602:GOL:O1	1.96	0.71
1:B:399:THR:OG1	1:B:528:GLU:OE2	2.05	0.71
1:C:278:ARG:NE	1:C:283:GLU:OE2	2.19	0.71
1:B:186:GLU:HG2	1:B:339:ASN:HB3	1.74	0.70
1:C:434:GLY:HA3	1:C:521:MET:HE3	1.74	0.69
1:C:235:PRO:HB2	1:C:306:HIS:CE1	2.28	0.69
1:C:404:ARG:NH1	5:C:604:JYD:O09	2.26	0.68
1:D:404:ARG:HD3	1:D:521:MET:CE	2.23	0.68
1:A:354:GLN:HG3	4:A:609:1PE:H151	1.77	0.67
1:A:227:MET:HE3	1:A:324:ILE:HD11	1.75	0.66
1:A:10:ALA:O	1:B:145:TYR:OH	2.12	0.66
1:B:227:MET:HE3	1:B:324:ILE:HD11	1.78	0.66
1:B:198:SER:HB3	1:B:328:CYS:HB3	1.80	0.64
1:D:237:HIS:HB2	1:D:327:SER:HB3	1.80	0.63
1:D:404:ARG:NH1	1:D:521:MET:HE1	2.13	0.63
1:C:181:ALA:HB1	1:D:126:ARG:CZ	2.28	0.63
1:D:19:SER:HB3	1:D:273:THR:O	1.99	0.62
1:A:186:GLU:HG2	1:A:339:ASN:HB3	1.80	0.62
1:C:31:LEU:HD13	1:C:343:VAL:HG12	1.82	0.62
1:C:109:ARG:NH2	1:C:350:MET:SD	2.73	0.62
1:C:26:THR:HG21	1:C:335:LEU:HD12	1.81	0.61
1:D:410:ARG:HD2	1:D:516:MET:SD	2.40	0.61
1:D:516:MET:HG3	1:D:524:VAL:HG23	1.82	0.61
1:A:161[B]:LEU:HD13	1:B:271:MET:HE3	1.82	0.60
1:D:378:MET:HE1	1:D:429:PRO:HD3	1.83	0.60
1:A:161[A]:LEU:HD23	1:B:271:MET:HE3	1.83	0.60
1:B:250:THR:HG22	1:B:251:MET:HE2	1.84	0.60
1:D:80:ARG:HD3	1:D:355:TYR:O	2.01	0.60
1:B:499:PRO:HB2	1:B:502:VAL:HG22	1.86	0.58
1:D:145:TYR:O	1:D:149[A]:GLN:HG2	2.03	0.58
1:C:36:VAL:CG1	1:C:49:LEU:HD11	2.33	0.58
1:A:521:MET:SD	1:A:522:GLU:HG2	2.44	0.58
1:D:541:LYS:NZ	6:D:715:HOH:O	2.36	0.58
1:C:50:ARG:NH1	1:D:44:GLY:HA3	2.19	0.57
1:C:249:MET:HE2	1:D:176:GLN:HG3	1.85	0.57
1:D:489:GLY:HA2	1:D:540:ASP:HB2	1.86	0.57
1:A:355:TYR:OH	6:A:701:HOH:O	2.11	0.57
1:C:61:SER:O	1:C:65:ASP:HB2	2.04	0.57
1:D:374:LEU:HD11	1:D:396:LEU:HB3	1.85	0.57
1:D:452:ALA:HB2	1:D:473:ALA:HB3	1.86	0.57
1:A:288:LYS:HD3	6:A:709:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HD23	1:A:310:VAL:HG11	1.87	0.57
1:A:26:THR:HG21	1:A:335:LEU:HD12	1.86	0.56
1:C:515:ASP:HB3	1:C:524:VAL:HB	1.87	0.56
1:A:424:TYR:OH	1:A:515:ASP:OD2	2.15	0.56
1:B:11:GLU:OE2	1:B:12:PHE:N	2.33	0.56
1:D:402:VAL:HB	1:D:525:TRP:HB2	1.88	0.56
1:D:215:LYS:NZ	1:D:219:ASN:OD1	2.25	0.56
1:D:94:PHE:O	1:D:98:GLN:HG2	2.06	0.56
1:D:492:TYR:HB3	1:D:538:VAL:HB	1.88	0.55
1:C:271:MET:HE3	1:D:161:LEU:HD23	1.88	0.55
1:C:421:LEU:HD12	1:C:422:PRO:HD2	1.89	0.55
1:B:452:ALA:HB2	1:B:473:ALA:HB3	1.88	0.55
1:C:36:VAL:HG11	1:C:339:ASN:O	2.07	0.55
1:A:105:ILE:HD12	1:A:502:VAL:HG12	1.89	0.55
1:C:282:LEU:HD12	1:C:310:VAL:HG21	1.89	0.54
1:D:154:ARG:HD2	1:D:521:MET:SD	2.47	0.54
1:D:518[A]:ASP:OD1	1:D:518[A]:ASP:N	2.40	0.54
1:B:229:GLY:O	1:B:236:TYR:OH	2.24	0.54
1:C:452:ALA:HB2	1:C:473:ALA:HB3	1.90	0.54
1:B:90:ASP:OD1	6:B:702:HOH:O	2.19	0.53
1:B:402:VAL:HB	1:B:525:TRP:HB2	1.91	0.53
1:B:11:GLU:CD	1:B:12:PHE:H	2.15	0.53
1:C:230:THR:HG23	1:C:295:MET:HE2	1.89	0.53
1:B:11:GLU:CD	1:B:12:PHE:N	2.67	0.53
1:D:205:LEU:HD22	1:D:224:LYS:HE3	1.91	0.53
1:C:129:GLN:NE2	6:C:722:HOH:O	2.41	0.52
1:C:269:PRO:HG3	1:C:277:PHE:CD1	2.44	0.52
1:B:315:ARG:HD2	1:B:319:SER:O	2.09	0.52
1:B:478:SER:OG	1:B:480:GLN:HG2	2.10	0.52
1:C:483:LYS:HD3	1:C:483:LYS:O	2.09	0.52
1:B:204:LEU:HD13	1:B:251:MET:HE3	1.92	0.52
1:A:19:SER:HB3	1:A:273:THR:O	2.10	0.52
1:C:217:LEU:HD21	1:D:163:MET:HE3	1.90	0.52
1:D:373:ASN:O	1:D:376:ARG:HD3	2.09	0.52
1:B:218:ARG:NH1	1:B:222:LYS:HZ3	2.07	0.52
1:D:17:LEU:HD13	1:D:249:MET:HE2	1.92	0.52
1:C:315:ARG:HD2	1:C:319:SER:O	2.10	0.52
1:D:537:VAL:HA	1:D:545:PHE:HB2	1.91	0.52
1:D:404:ARG:HD3	1:D:521:MET:HE1	1.89	0.51
1:C:64:PHE:HA	1:C:67:VAL:HG22	1.92	0.51
1:B:94:PHE:O	1:B:98:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LYS:HD3	1:C:315:ARG:NH2	2.26	0.51
1:C:450:THR:HG23	1:C:454:ARG:NH1	2.26	0.51
1:D:146:ASP:OD2	6:D:701:HOH:O	2.19	0.51
1:B:512:GLU:OE2	1:B:526:ARG:HB3	2.11	0.50
1:A:71:LEU:HD13	1:A:75:HIS:CD2	2.47	0.50
1:A:69:HIS:CD2	1:A:109:ARG:HA	2.47	0.50
1:C:102:ASN:CG	1:C:499:PRO:HA	2.37	0.50
1:C:469:MET:HE1	1:C:488:TYR:O	2.12	0.50
1:C:72:ARG:HD2	6:C:705:HOH:O	2.11	0.50
1:C:405:ASP:OD2	6:C:701:HOH:O	2.19	0.50
1:D:390:VAL:HG12	1:D:536:ILE:HG22	1.92	0.50
1:A:478:SER:OG	1:A:480:GLN:HG2	2.13	0.49
1:C:214:PRO:O	1:C:218[B]:ARG:HG2	2.12	0.49
1:C:36:VAL:HG12	1:C:49:LEU:HD11	1.93	0.49
1:C:197:GLY:O	1:C:201[B]:LYS:HG2	2.12	0.49
1:B:499:PRO:O	1:B:502:VAL:HG22	2.13	0.49
1:B:251:MET:HE1	1:B:323:GLY:CA	2.43	0.49
1:C:394:LEU:HD11	1:C:536:ILE:HG13	1.93	0.49
1:D:33:LYS:CD	4:D:603:1PE:H222	2.40	0.49
1:D:89:SER:O	1:D:92:ASP:HB2	2.13	0.49
1:D:229:GLY:HA2	1:D:295:MET:HE1	1.94	0.49
1:D:352:PRO:HG3	6:D:823:HOH:O	2.13	0.49
1:C:378:MET:HE1	1:C:429:PRO:HD3	1.95	0.49
1:C:201[A]:LYS:HE2	1:C:231:SER:HB2	1.94	0.49
1:C:374:LEU:HD11	1:C:396:LEU:HB3	1.94	0.49
1:B:104:ASN:OD1	1:B:353:SER:HB3	2.13	0.48
1:C:376:ARG:HB2	1:C:380[A]:GLU:HG2	1.95	0.48
1:B:400:ILE:HG21	1:B:431:TYR:HB2	1.94	0.48
1:C:451:THR:OG1	5:C:604:JYD:O05	2.28	0.48
1:B:391:ARG:HG2	1:B:545:PHE:CE2	2.48	0.48
1:D:154:ARG:CZ	1:D:521:MET:SD	3.01	0.48
1:A:181:ALA:HB1	1:B:126:ARG:NH2	2.28	0.48
1:A:248:GLU:OE2	1:B:255:LYS:NZ	2.42	0.48
1:B:509:LYS:NZ	6:B:722:HOH:O	2.40	0.48
1:A:154:ARG:NH1	5:A:608[B]:JYD:O09	2.26	0.48
1:B:80:ARG:HD3	1:B:355:TYR:O	2.12	0.48
1:A:447:PHE:HB3	1:A:508:ILE:HD13	1.95	0.48
1:A:136:ASP:OD2	1:A:187:TYR:OH	2.20	0.48
1:D:41:PRO:HG2	1:D:45:LEU:HB2	1.95	0.47
1:B:69:HIS:CD2	1:B:109:ARG:HA	2.49	0.47
1:A:492:TYR:HB3	1:A:538:VAL:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:GLU:O	1:C:285:GLU:HG2	2.14	0.47
1:A:487:LYS:HD2	1:A:488:TYR:CE2	2.50	0.47
1:C:269:PRO:HG3	1:C:277:PHE:CE1	2.49	0.47
1:C:316:HIS:HE2	1:D:116:ASP:CG	2.22	0.47
1:B:128:ASP:HB2	1:B:183:LYS:HA	1.97	0.47
1:C:447:PHE:HB3	1:C:508:ILE:HD13	1.96	0.47
4:A:609:1PE:H132	4:A:609:1PE:H222	1.60	0.47
1:D:64:PHE:HA	1:D:67:VAL:HG22	1.96	0.47
1:C:284:GLU:O	1:C:288:LYS:HD3	2.15	0.47
1:D:201:LYS:HE3	1:D:231:SER:HB2	1.96	0.47
1:A:515:ASP:HB3	1:A:524:VAL:HB	1.97	0.47
1:B:169:THR:O	6:B:703:HOH:O	2.21	0.47
1:C:278:ARG:NH2	1:C:283:GLU:OE1	2.48	0.47
1:A:499:PRO:O	1:A:502:VAL:HG22	2.15	0.46
1:C:28:TYR:HB3	1:C:344:TRP:HB3	1.96	0.46
1:D:49:LEU:N	1:D:129:GLN:O	2.38	0.46
1:C:12:PHE:CZ	1:C:14:PHE:HB2	2.50	0.46
1:C:293:ILE:HG22	6:C:763:HOH:O	2.15	0.46
1:C:415:LEU:HD21	1:C:421:LEU:HB2	1.96	0.46
1:C:288:LYS:HD2	1:C:288:LYS:N	2.30	0.46
1:B:415:LEU:HD13	1:B:465:HIS:CD2	2.50	0.46
1:C:98:GLN:HG3	1:C:496:ILE:HD13	1.96	0.46
1:D:224:LYS:NZ	6:D:705:HOH:O	2.27	0.46
1:D:229:GLY:O	1:D:236:TYR:OH	2.18	0.46
1:A:21:VAL:HG12	1:A:22:SER:O	2.16	0.46
1:C:88:ALA:HB2	1:C:303:TYR:HE2	1.81	0.46
1:A:102:ASN:CG	1:A:499:PRO:HA	2.41	0.46
1:A:512:GLU:HG2	1:A:526:ARG:O	2.16	0.46
1:D:471:MET:SD	1:D:477:ARG:NH1	2.84	0.46
1:B:197:GLY:N	5:B:604[B]:JYD:S06	2.87	0.46
1:C:383:GLN:O	1:C:387:LYS:HG3	2.16	0.46
1:C:463:GLN:HA	1:C:467:GLY:O	2.16	0.45
1:A:222:LYS:HE3	1:A:222:LYS:HB2	1.62	0.45
1:A:447:PHE:HB3	1:A:508:ILE:CD1	2.47	0.45
4:A:611:1PE:H131	4:A:611:1PE:H141	1.60	0.45
1:C:540:ASP:OD2	1:C:541:LYS:NZ	2.37	0.45
1:A:404:ARG:NH1	5:A:608[B]:JYD:O08	2.48	0.45
1:D:101:LYS:HB2	1:D:101:LYS:HE3	1.79	0.45
1:C:386:SER:OG	1:C:540:ASP:OD1	2.18	0.45
1:A:142:ARG:NH1	6:A:719:HOH:O	2.39	0.45
1:C:232:ALA:HB3	1:C:236:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:515:ASP:HB3	1:D:524:VAL:HB	1.97	0.45
1:C:29:ARG:NH1	6:C:713:HOH:O	2.33	0.45
1:A:450:THR:HG23	5:A:608[B]:JYD:O04	2.17	0.45
1:A:291:GLN:HE22	3:A:603:GOL:H2	1.82	0.45
1:C:200:ASN:ND2	1:D:318:ALA:O	2.50	0.45
1:D:116:ASP:HB2	5:D:602:JYD:C07	2.47	0.45
4:B:606:1PE:H131	6:B:774:HOH:O	2.16	0.45
1:C:372:VAL:HG21	1:C:394:LEU:HD23	1.98	0.45
1:C:401:ILE:HD13	1:C:401:ILE:HA	1.72	0.45
1:C:42:GLY:N	1:D:41:PRO:O	2.36	0.44
1:A:23:HIS:HB2	3:A:602:GOL:O2	2.17	0.44
1:D:33:LYS:HD2	4:D:603:1PE:H232	1.99	0.44
1:B:415:LEU:HD23	1:B:419:LYS:O	2.17	0.44
1:B:237:HIS:HB2	1:B:327:SER:HB3	1.98	0.44
1:B:410:ARG:O	1:B:414:MET:HG3	2.18	0.44
1:C:435:PRO:HB3	1:C:447:PHE:CD2	2.52	0.44
1:B:275:TYR:HB3	1:B:314:PRO:HG3	2.00	0.44
1:B:499:PRO:HB2	1:B:502:VAL:CG2	2.48	0.44
1:D:51:VAL:O	1:D:133:PRO:HD2	2.18	0.44
1:B:404:ARG:HH12	5:B:604[A]:JYD:C07	2.30	0.44
1:C:45:LEU:HD11	1:D:48:MET:HG3	2.00	0.44
1:B:447:PHE:HB3	1:B:508:ILE:CD1	2.47	0.44
1:C:447:PHE:HB3	1:C:508:ILE:CD1	2.48	0.43
1:D:315:ARG:HD2	1:D:319:SER:O	2.18	0.43
1:B:351:GLU:O	1:B:354:GLN:HG2	2.19	0.43
1:D:71:LEU:HD23	1:D:75:HIS:CD2	2.54	0.43
1:B:268:LYS:HD3	1:B:268:LYS:HA	1.44	0.43
1:C:282:LEU:HD12	1:C:310:VAL:CG2	2.49	0.43
1:C:392:THR:HB	1:C:536:ILE:HD12	2.00	0.43
1:D:483:LYS:O	1:D:487:LYS:HB2	2.18	0.43
1:A:235:PRO:HB2	1:A:306:HIS:CE1	2.53	0.43
4:C:605:1PE:H142	4:C:605:1PE:H152	1.85	0.43
1:B:204:LEU:CD1	1:B:251:MET:HE3	2.48	0.43
1:B:209:LYS:HD3	1:B:315:ARG:NH2	2.33	0.43
1:A:64:PHE:HA	1:A:67:VAL:HG22	1.99	0.43
1:A:100:LEU:HB3	1:A:356:LEU:HD13	2.01	0.43
1:C:81:LYS:HD2	4:C:606:1PE:H231	2.00	0.43
1:D:289:VAL:O	6:D:703:HOH:O	2.22	0.43
1:D:451:THR:N	1:D:474:LYS:HE3	2.34	0.43
1:B:190:MET:HE3	1:B:335:LEU:HD21	2.01	0.43
1:B:472:LEU:HA	1:B:493:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ALA:O	1:C:189:PHE:HA	2.19	0.42
1:C:215:LYS:HG3	3:C:602:GOL:H11	2.00	0.42
1:D:500:ALA:HB2	6:D:782:HOH:O	2.18	0.42
1:B:16:PRO:HG2	1:B:273:THR:O	2.19	0.42
1:A:71:LEU:HD13	1:A:75:HIS:HD2	1.84	0.42
1:A:415:LEU:HD13	1:A:465:HIS:CD2	2.55	0.42
1:C:45:LEU:HA	1:C:46:PRO:HD3	1.93	0.42
1:B:33:LYS:HE3	4:B:605:1PE:H142	2.02	0.42
1:C:82:ILE:HG12	1:C:303:TYR:CZ	2.54	0.42
1:C:161:LEU:C	1:D:269:PRO:HG2	2.45	0.42
1:B:129:GLN:CB	1:B:185:MET:HG3	2.50	0.42
1:B:208:THR:O	1:B:211:VAL:HG12	2.19	0.42
1:B:218:ARG:HH11	1:B:222:LYS:HZ3	1.66	0.42
1:C:376:ARG:CB	1:C:380[A]:GLU:HG2	2.49	0.42
1:D:225:LEU:HD11	1:D:286:VAL:HG13	2.01	0.42
1:C:68:GLU:HG3	1:C:153:PHE:CZ	2.55	0.42
1:D:521:MET:HG3	1:D:522:GLU:N	2.33	0.42
1:A:346:GLU:O	6:A:702:HOH:O	2.21	0.42
1:B:447:PHE:HB3	1:B:508:ILE:HD13	2.02	0.42
1:C:128:ASP:OD1	1:C:183:LYS:HA	2.19	0.42
1:C:284:GLU:OE1	4:C:605:1PE:OH6	2.38	0.41
1:D:106:SER:HB2	1:D:111:LEU:O	2.20	0.41
1:B:33:LYS:CE	4:B:605:1PE:H131	2.50	0.41
1:B:234:PRO:HD2	1:B:298:GLN:HG2	2.01	0.41
1:B:391:ARG:HB3	1:B:391:ARG:HH11	1.86	0.41
1:C:411:MET:HG3	1:C:516:MET:HE1	2.02	0.41
1:A:197:GLY:HA3	5:A:608[A]:JYD:O05	2.21	0.41
1:D:384:GLU:OE1	1:D:387:LYS:NZ	2.48	0.41
1:C:89:SER:O	1:C:93:LYS:HG3	2.21	0.41
1:C:216:SER:HA	3:C:602:GOL:O1	2.20	0.41
1:B:373:ASN:O	1:B:376:ARG:NE	2.51	0.41
1:B:400:ILE:HG12	1:B:429:PRO:HB2	2.03	0.41
1:A:449:PRO:HG2	1:A:474:LYS:HG2	2.03	0.41
3:C:602:GOL:O1	3:C:602:GOL:O3	2.23	0.41
1:A:19:SER:HB3	1:A:273:THR:C	2.46	0.41
1:D:19:SER:HB3	1:D:273:THR:C	2.46	0.41
1:D:404:ARG:CZ	1:D:521:MET:HE1	2.50	0.41
1:B:270:ASP:OD2	1:B:273:THR:HG23	2.20	0.41
1:B:48:MET:CE	6:B:910:HOH:O	2.56	0.41
1:C:248:GLU:H	1:C:248:GLU:CD	2.29	0.41
1:C:354:GLN:OE1	4:C:603:1PE:OH4	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:VAL:HG13	1:C:527:ILE:HG22	2.03	0.41
1:D:45:LEU:HA	1:D:46:PRO:HD3	1.95	0.41
1:B:102:ASN:CG	1:B:499:PRO:HA	2.45	0.41
1:B:477:ARG:HD3	1:B:481:VAL:HG11	2.03	0.41
1:C:82:ILE:HG12	1:C:303:TYR:CE2	2.56	0.41
1:D:402:VAL:O	1:D:524:VAL:HA	2.21	0.41
1:C:471:MET:HE3	1:C:471:MET:HB2	1.93	0.40
1:D:390:VAL:HA	1:D:536:ILE:HB	2.03	0.40
1:A:151:ARG:HH12	3:A:604:GOL:H32	1.85	0.40
1:A:376:ARG:HA	1:A:376:ARG:HD2	1.89	0.40
1:B:128:ASP:OD2	6:B:704:HOH:O	2.22	0.40
1:D:157:GLN:HG2	1:D:172:ASN:OD1	2.20	0.40
1:D:389:PRO:O	1:D:392:THR:OG1	2.28	0.40
1:A:426:LYS:HE2	1:A:465:HIS:O	2.21	0.40
1:B:64:PHE:O	1:B:68:GLU:HG2	2.22	0.40
1:C:424:TYR:CE1	1:C:524:VAL:HG11	2.55	0.40

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%)	43	38
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%)	442 (99%)	3 (1%)	76	79
1	B	446/491 (91%)	442 (99%)	4 (1%)	70	74
1	C	428/491 (87%)	422 (99%)	6 (1%)	59	60
1	D	421/491 (86%)	415 (99%)	6 (1%)	59	60
All	All	1740/1964 (89%)	1721 (99%)	19 (1%)	70	68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	LEU
1	A	493	LEU
1	A	512	GLU
1	B	21	VAL
1	B	282	LEU
1	B	521[A]	MET
1	B	521[B]	MET
1	C	15	VAL
1	C	367	THR
1	C	380[A]	GLU
1	C	380[B]	GLU
1	C	401	ILE
1	C	521	MET
1	D	15	VAL
1	D	149[A]	GLN
1	D	149[B]	GLN
1	D	282	LEU
1	D	518[A]	ASP
1	D	518[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	158	ASN
1	B	463	GLN
1	C	172	ASN
1	C	486	HIS
1	C	531	ASN
1	D	23	HIS
1	D	69	HIS
1	D	333	GLN
1	D	463	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
4	1PE	A	611	-	9,9,15	0.29	0	8,8,14	0.39	0
4	1PE	C	603	-	6,6,15	0.51	0	5,5,14	0.37	0
2	SF4	C	601	1,5	0,12,12	-	-	-		
3	GOL	A	606	-	5,5,5	1.18	1 (20%)	5,5,5	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	602	-	5,5,5	0.92	0	5,5,5	1.13	0
4	1PE	A	609	-	12,12,15	0.52	0	11,11,14	0.60	0
2	SF4	A	601	1,5	0,12,12	-	-	-		
3	GOL	B	603	-	5,5,5	1.21	1 (20%)	5,5,5	1.18	0
2	SF4	B	601	1,5	0,12,12	-	-	-		
4	1PE	C	606	-	9,9,15	0.27	0	8,8,14	0.50	0
2	SF4	D	601	1,5	0,12,12	-	-	-		
4	1PE	A	607	-	6,6,15	0.52	0	5,5,14	0.38	0
3	GOL	B	602	-	5,5,5	0.87	0	5,5,5	1.67	1 (20%)
4	1PE	B	605	-	12,12,15	0.56	0	11,11,14	0.66	0
4	1PE	B	606	-	9,9,15	0.30	0	8,8,14	0.40	0
5	JYD	B	604[A]	2	6,8,8	1.14	0	7,10,10	1.57	1 (14%)
5	JYD	A	608[A]	2	6,8,8	1.14	0	7,10,10	1.40	1 (14%)
5	JYD	B	604[B]	2	6,8,8	1.17	0	7,10,10	1.16	0
5	JYD	A	608[B]	2	6,8,8	1.19	0	7,10,10	1.41	2 (28%)
5	JYD	C	604	2	6,8,8	1.18	0	7,10,10	1.21	0
4	1PE	D	603	-	15,15,15	0.56	0	14,14,14	0.38	0
4	1PE	A	610	-	9,9,15	0.36	0	8,8,14	0.35	0
4	1PE	C	605	-	9,9,15	0.28	0	8,8,14	0.49	0
3	GOL	A	602	-	5,5,5	1.78	1 (20%)	5,5,5	1.17	1 (20%)
3	GOL	A	604	-	5,5,5	1.19	1 (20%)	5,5,5	1.19	0
5	JYD	D	602	2	6,8,8	1.06	0	7,10,10	1.84	3 (42%)
3	GOL	A	603	-	5,5,5	1.33	1 (20%)	5,5,5	1.01	0
3	GOL	A	605	-	5,5,5	1.34	1 (20%)	5,5,5	0.87	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
4	1PE	A	611	-	-	5/7/7/13	-
4	1PE	C	603	-	-	4/4/4/13	-
2	SF4	C	601	1,5	-	-	0/6/5/5
3	GOL	A	606	-	-	2/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
4	1PE	A	609	-	-	7/10/10/13	-
2	SF4	A	601	1,5	-	-	0/6/5/5
3	GOL	B	603	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	601	1,5	-	-	0/6/5/5
4	1PE	C	606	-	-	3/7/7/13	-
2	SF4	D	601	1,5	-	-	0/6/5/5
4	1PE	A	607	-	-	1/4/4/13	-
3	GOL	B	602	-	-	4/4/4/4	-
4	1PE	B	605	-	-	2/10/10/13	-
4	1PE	B	606	-	-	4/7/7/13	-
5	JYD	B	604[A]	2	-	1/6/8/8	-
5	JYD	A	608[A]	2	-	1/6/8/8	-
5	JYD	B	604[B]	2	-	2/6/8/8	-
5	JYD	A	608[B]	2	-	1/6/8/8	-
5	JYD	C	604	2	-	2/6/8/8	-
4	1PE	D	603	-	-	11/13/13/13	-
4	1PE	A	610	-	-	5/7/7/13	-
4	1PE	C	605	-	-	3/7/7/13	-
3	GOL	A	602	-	-	0/4/4/4	-
3	GOL	A	604	-	-	4/4/4/4	-
5	JYD	D	602	2	-	2/6/8/8	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	A	605	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	GOL	O2-C2	-3.41	1.33	1.43
3	A	605	GOL	O2-C2	-2.84	1.35	1.43
3	A	603	GOL	O2-C2	-2.77	1.35	1.43
3	B	603	GOL	O2-C2	-2.38	1.36	1.43
3	A	606	GOL	O2-C2	-2.15	1.37	1.43
3	A	604	GOL	O2-C2	-2.11	1.37	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	GOL	C3-C2-C1	-2.81	101.50	111.80
5	D	602	JYD	O09-C07-C01	2.75	122.54	114.00
5	D	602	JYD	O08-C07-C01	-2.59	114.89	122.84
5	B	604[A]	JYD	C01-C02-C03	-2.57	108.08	112.98
5	D	602	JYD	O04-C03-C02	2.34	120.47	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	GOL	C3-C2-C1	-2.19	103.76	111.80
5	A	608[B]	JYD	O04-C03-C02	2.06	119.71	114.00
5	A	608[A]	JYD	O04-C03-C02	2.02	119.60	114.00
5	A	608[B]	JYD	O09-C07-C01	2.00	120.23	114.00

There are no chirality outliers.

All (70) 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
5	A	608[B]	JYD	C07-C01-C02-C03
5	B	604[A]	JYD	C07-C01-C02-S06
5	B	604[B]	JYD	C07-C01-C02-C03
5	B	604[B]	JYD	C07-C01-C02-S06
5	C	604	JYD	C07-C01-C02-S06
5	D	602	JYD	C07-C01-C02-S06
4	A	609	1PE	C13-C23-OH3-C22
4	B	605	1PE	OH4-C13-C23-OH3
4	A	609	1PE	OH5-C14-C24-OH4
4	C	606	1PE	OH5-C14-C24-OH4
4	A	611	1PE	C14-C24-OH4-C13
4	D	603	1PE	OH4-C13-C23-OH3
4	A	609	1PE	OH4-C13-C23-OH3
4	A	610	1PE	OH5-C14-C24-OH4
3	C	602	GOL	O1-C1-C2-O2
4	A	607	1PE	OH4-C13-C23-OH3
4	B	606	1PE	OH5-C14-C24-OH4
4	D	603	1PE	OH2-C12-C22-OH3
3	A	605	GOL	O1-C1-C2-C3
3	B	602	GOL	O1-C1-C2-C3
3	B	602	GOL	C1-C2-C3-O3
4	A	610	1PE	OH6-C15-C25-OH5
4	C	603	1PE	OH4-C13-C23-OH3
4	D	603	1PE	OH7-C16-C26-OH6
3	A	603	GOL	O1-C1-C2-O2
3	A	604	GOL	O1-C1-C2-O2
3	A	606	GOL	O2-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	D	603	1PE	OH5-C14-C24-OH4
4	A	611	1PE	OH4-C13-C23-OH3
5	D	602	JYD	C07-C01-C02-C03
4	B	606	1PE	OH4-C13-C23-OH3
4	C	606	1PE	C24-C14-OH5-C25
4	D	603	1PE	OH6-C15-C25-OH5
5	C	604	JYD	C07-C01-C02-C03
4	C	603	1PE	OH2-C12-C22-OH3
4	C	606	1PE	OH4-C13-C23-OH3
3	A	604	GOL	O2-C2-C3-O3
4	C	605	1PE	C15-C25-OH5-C14
4	A	609	1PE	C24-C14-OH5-C25
4	A	610	1PE	C23-C13-OH4-C24
3	A	604	GOL	C1-C2-C3-O3
4	C	605	1PE	C23-C13-OH4-C24
4	A	610	1PE	C24-C14-OH5-C25
4	C	603	1PE	C13-C23-OH3-C22
4	A	609	1PE	OH2-C12-C22-OH3
4	B	605	1PE	OH2-C12-C22-OH3
4	B	606	1PE	C14-C24-OH4-C13
4	A	611	1PE	OH6-C15-C25-OH5
4	B	606	1PE	C24-C14-OH5-C25
4	A	609	1PE	C14-C24-OH4-C13
4	A	610	1PE	C14-C24-OH4-C13
4	D	603	1PE	C25-C15-OH6-C26
4	C	603	1PE	C12-C22-OH3-C23
4	D	603	1PE	C24-C14-OH5-C25
4	D	603	1PE	C12-C22-OH3-C23
4	D	603	1PE	C23-C13-OH4-C24
4	D	603	1PE	C13-C23-OH3-C22
4	A	609	1PE	OH6-C15-C25-OH5
4	A	611	1PE	OH5-C14-C24-OH4
4	C	605	1PE	OH6-C15-C25-OH5
3	A	605	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-O2
4	D	603	1PE	C16-C26-OH6-C15
4	A	611	1PE	C15-C25-OH5-C14

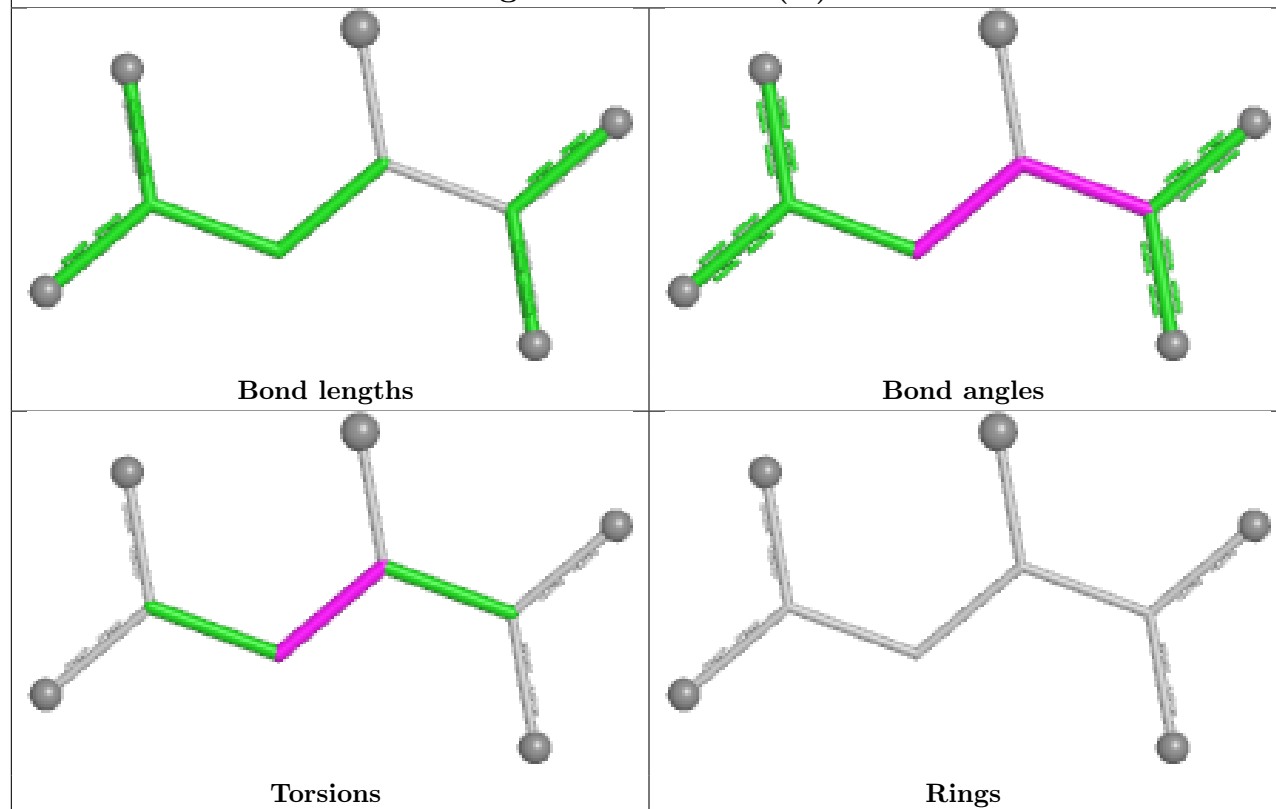
There are no ring outliers.

20 monomers are involved in 31 short contacts:

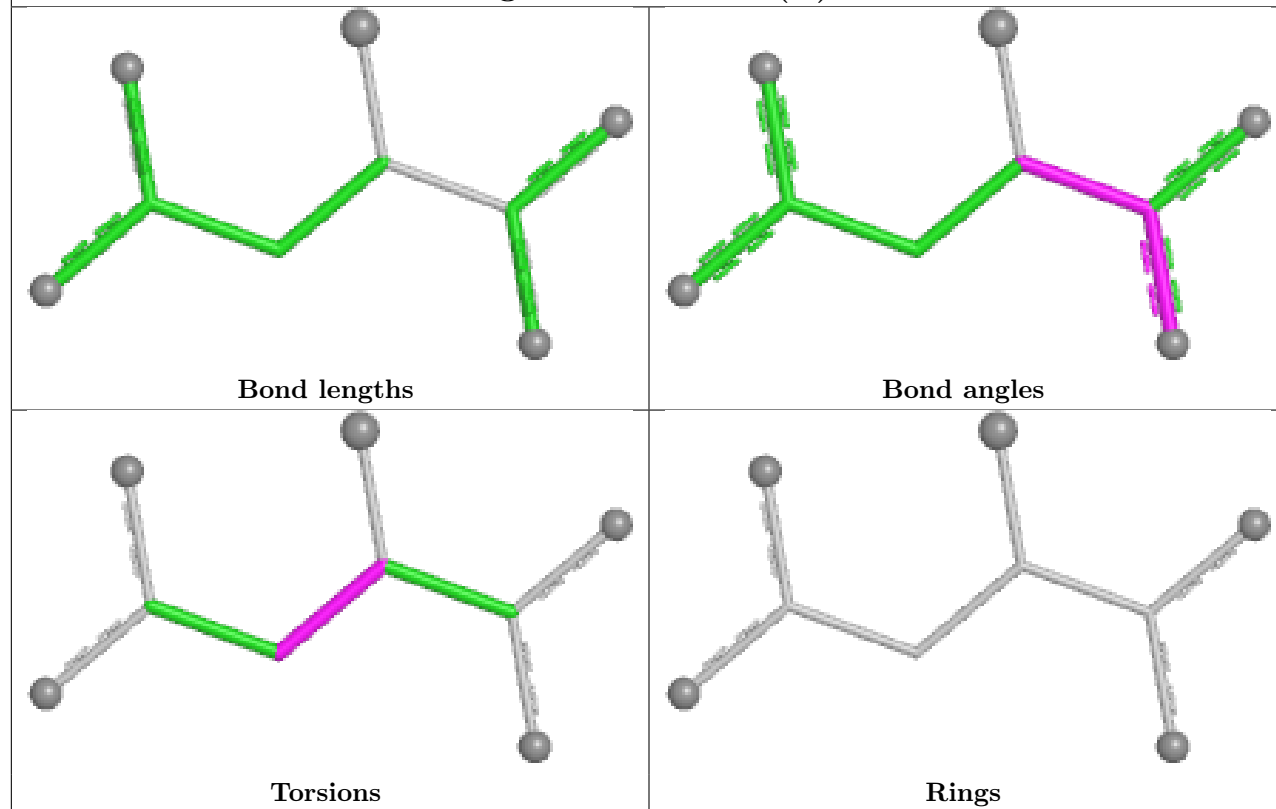
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	611	1PE	1	0
4	C	603	1PE	1	0
3	C	602	GOL	3	0
4	A	609	1PE	2	0
4	C	606	1PE	1	0
3	B	602	GOL	1	0
4	B	605	1PE	2	0
4	B	606	1PE	1	0
5	B	604[A]	JYD	1	0
5	A	608[A]	JYD	1	0
5	B	604[B]	JYD	1	0
5	A	608[B]	JYD	3	0
5	C	604	JYD	2	0
4	D	603	1PE	4	0
4	A	610	1PE	1	0
4	C	605	1PE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

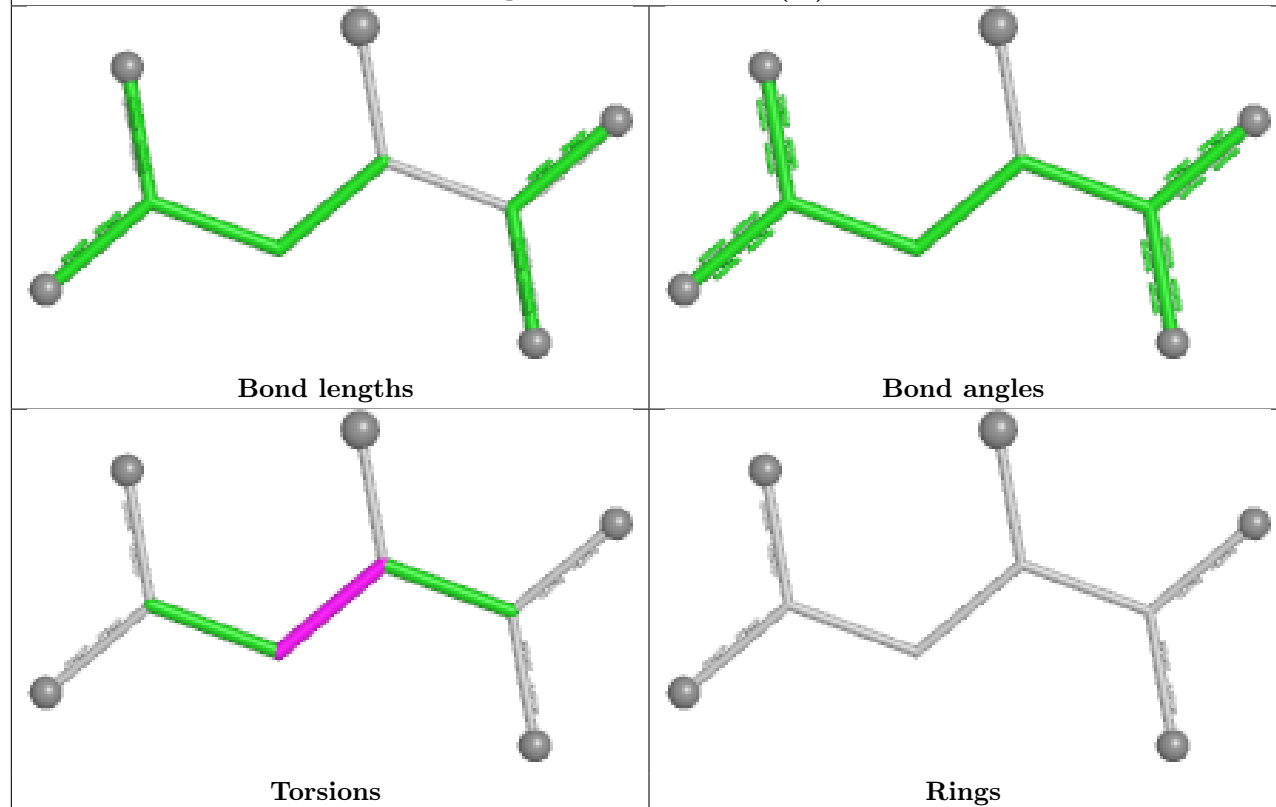
Ligand JYD B 604 (A)



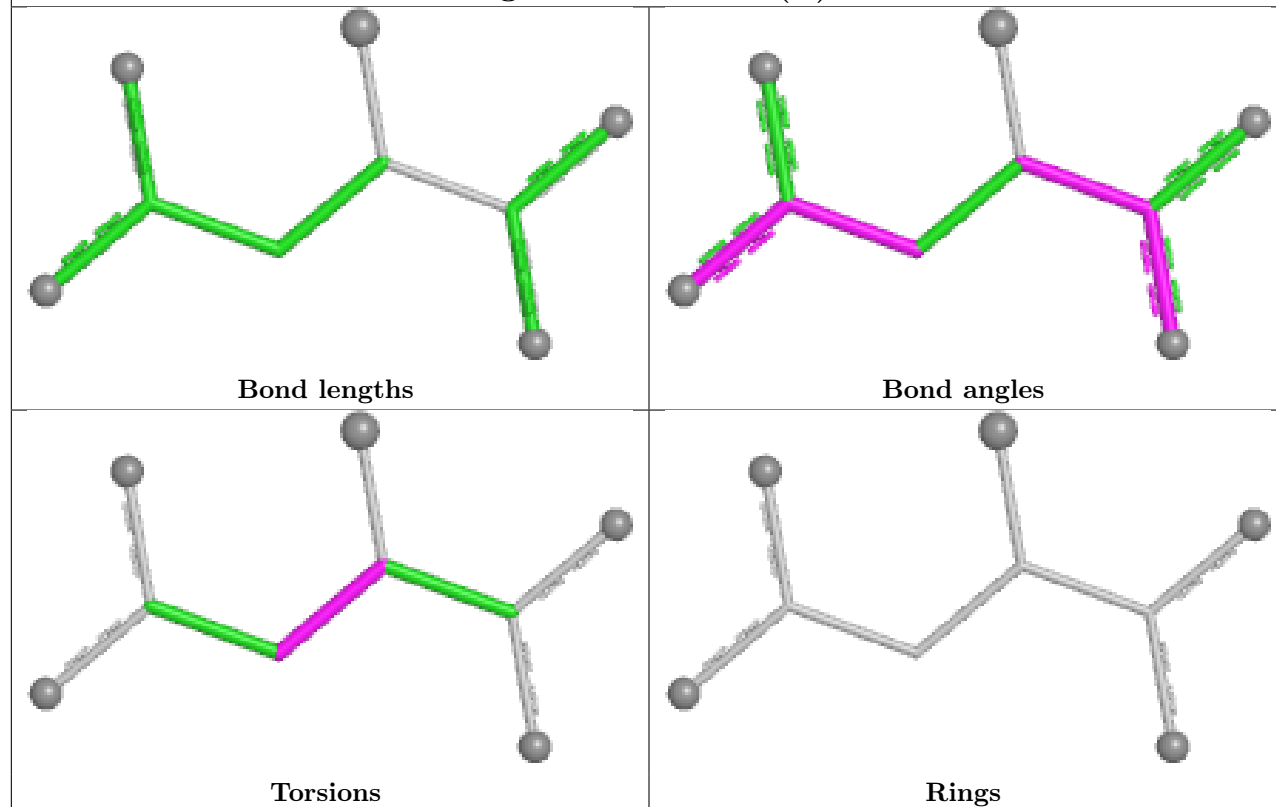
Ligand JYD A 608 (A)



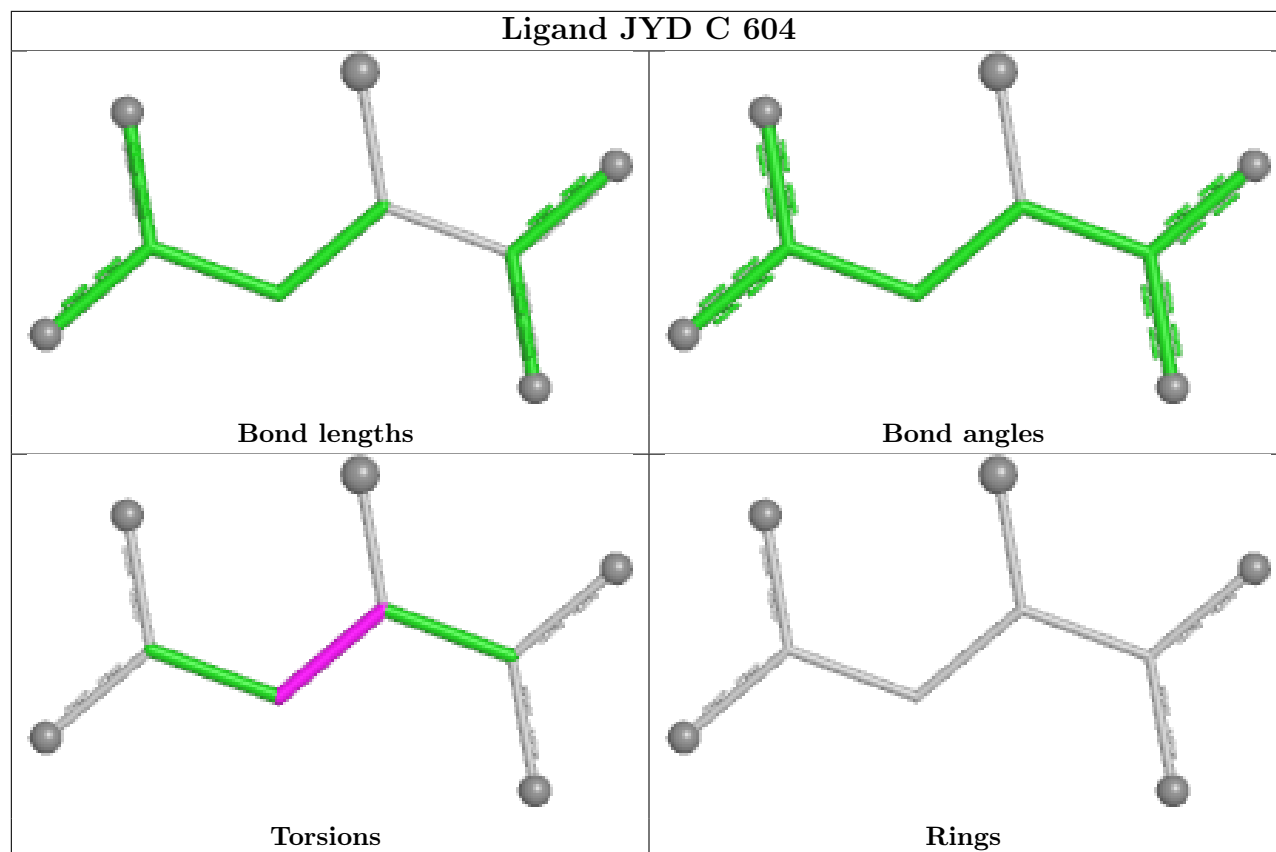
Ligand JYD B 604 (B)



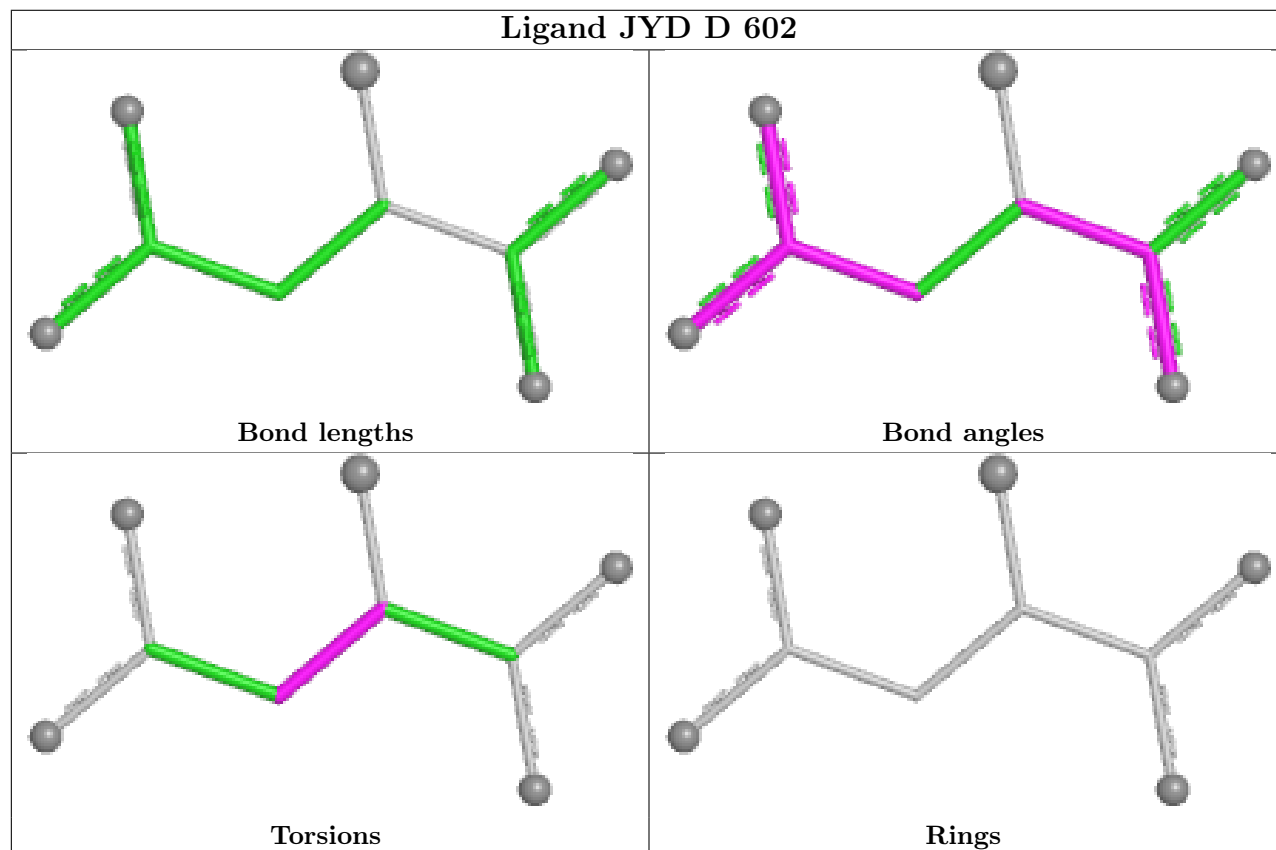
Ligand JYD A 608 (B)



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

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	540/585 (92%)	0.65	34 (6%)	26 25	9, 20, 34, 51	3 (0%)
1	B	540/585 (92%)	0.57	29 (5%)	31 31	9, 20, 37, 49	4 (0%)
1	C	528/585 (90%)	1.25	93 (17%)	4 3	13, 33, 47, 64	3 (0%)
1	D	531/585 (90%)	1.43	134 (25%)	1 1	13, 34, 55, 69	2 (0%)
All	All	2139/2340 (91%)	0.97	290 (13%)	7 6	9, 28, 48, 69	12 (0%)

All (290) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	325	GLY	4.9
1	D	372	VAL	4.7
1	D	390	VAL	4.7
1	A	301	GLY	4.3
1	C	318	ALA	4.2
1	D	441	GLY	4.2
1	D	466	GLY	4.1
1	D	38	VAL	4.0
1	D	243	GLY	4.0
1	C	220	PHE	4.0
1	D	543	ASN	3.9
1	A	54	ALA	3.9
1	A	67	VAL	3.9
1	C	545	PHE	3.9
1	C	73	SER	3.9
1	B	471[A]	MET	3.8
1	A	35	TYR	3.8
1	D	232	ALA	3.8
1	C	350	MET	3.8
1	C	45	LEU	3.7
1	B	258	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	97	LEU	3.7
1	D	542	GLY	3.7
1	B	441	GLY	3.6
1	D	406	SER	3.6
1	D	539	ASP	3.6
1	A	196	GLY	3.6
1	D	381	VAL	3.5
1	D	482	THR	3.5
1	B	250	THR	3.5
1	C	44	GLY	3.5
1	C	296	GLY	3.5
1	D	169	THR	3.5
1	D	445	GLY	3.4
1	C	46	PRO	3.4
1	C	447	PHE	3.3
1	D	417	ALA	3.3
1	C	348	LEU	3.3
1	C	131	PHE	3.3
1	B	358	ASP	3.3
1	D	197	GLY	3.3
1	D	379	PRO	3.3
1	D	136	ASP	3.3
1	D	467	GLY	3.2
1	C	303	TYR	3.2
1	D	228	PHE	3.2
1	C	127	GLY	3.2
1	D	303	TYR	3.2
1	D	218	ARG	3.2
1	C	535	PHE	3.2
1	C	155	TYR	3.1
1	D	468	SER	3.1
1	D	88	ALA	3.1
1	D	258	SER	3.1
1	D	545	PHE	3.1
1	D	358	ASP	3.1
1	C	310	VAL	3.1
1	D	304	TYR	3.0
1	C	352	PRO	3.0
1	D	247	ALA	3.0
1	D	407	ALA	3.0
1	C	481	VAL	3.0
1	D	236	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	86	PRO	3.0
1	C	218[A]	ARG	3.0
1	D	305	ALA	3.0
1	C	400	ILE	3.0
1	B	261	TYR	3.0
1	D	45	LEU	2.9
1	D	342	GLY	2.9
1	C	354	GLN	2.9
1	A	247	ALA	2.9
1	C	531	ASN	2.9
1	C	97	LEU	2.9
1	C	294	GLY	2.9
1	C	357	PRO	2.9
1	C	546	PHE	2.9
1	B	257	ALA	2.9
1	D	484	ALA	2.9
1	D	502	VAL	2.9
1	D	369	ALA	2.9
1	B	243	GLY	2.9
1	D	464	SER	2.8
1	D	14	PHE	2.8
1	D	491	PHE	2.8
1	D	488	TYR	2.8
1	A	36	VAL	2.8
1	D	524	VAL	2.8
1	B	220	PHE	2.8
1	C	143	GLY	2.8
1	D	370	VAL	2.8
1	B	322	ILE	2.8
1	B	61	SER	2.7
1	C	351	GLU	2.7
1	D	270	ASP	2.7
1	C	441	GLY	2.7
1	C	467	GLY	2.7
1	D	459	VAL	2.7
1	D	400	ILE	2.7
1	B	182	SER	2.7
1	D	532	PHE	2.7
1	D	256	TYR	2.7
1	C	384	GLU	2.7
1	C	529	VAL	2.7
1	D	86	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	435	PRO	2.7
1	A	242	ILE	2.7
1	A	536	ILE	2.7
1	D	344	TRP	2.7
1	B	442	LEU	2.6
1	D	397	THR	2.6
1	C	338	ILE	2.6
1	A	418	GLY	2.6
1	A	199	ALA	2.6
1	A	452	ALA	2.6
1	C	345	LEU	2.6
1	D	253	VAL	2.6
1	C	114	CYS	2.6
1	C	344	TRP	2.6
1	D	181	ALA	2.6
1	D	507	ALA	2.6
1	A	449	PRO	2.6
1	D	490	GLY	2.6
1	C	297	ALA	2.6
1	D	192	VAL	2.5
1	D	470	VAL	2.5
1	C	520	GLY	2.5
1	D	398	GLY	2.5
1	A	165	ASP	2.5
1	D	66	ASP	2.5
1	A	429	PRO	2.5
1	C	43	ALA	2.5
1	C	144	VAL	2.5
1	D	518[A]	ASP	2.5
1	C	500	ALA	2.5
1	C	287	LEU	2.5
1	D	546	PHE	2.5
1	C	509	LYS	2.5
1	D	536	ILE	2.5
1	D	373	ASN	2.5
1	D	261	TYR	2.5
1	C	32	THR	2.5
1	D	107	SER	2.5
1	D	392	THR	2.5
1	C	379	PRO	2.5
1	D	376	ARG	2.5
1	A	197	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	342	GLY	2.5
1	A	311	ILE	2.5
1	A	62	THR	2.4
1	D	161	LEU	2.4
1	C	390	VAL	2.4
1	D	165	ASP	2.4
1	D	322	ILE	2.4
1	C	295	MET	2.4
1	D	371	MET	2.4
1	B	330	ALA	2.4
1	C	27	LYS	2.4
1	B	382	LEU	2.4
1	C	30	LEU	2.4
1	C	31	LEU	2.4
1	B	286	VAL	2.4
1	D	144	VAL	2.4
1	D	290	CYS	2.4
1	D	429	PRO	2.4
1	D	221	LEU	2.4
1	D	385	LEU	2.4
1	D	493	LEU	2.4
1	D	13	ASN	2.4
1	A	537	VAL	2.4
1	C	502	VAL	2.4
1	D	21	VAL	2.4
1	B	444	SER	2.4
1	D	269	PRO	2.4
1	D	396	LEU	2.3
1	A	323	GLY	2.3
1	C	42	GLY	2.3
1	C	83	PHE	2.3
1	D	12	PHE	2.3
1	D	350	MET	2.3
1	D	130	VAL	2.3
1	C	26	THR	2.3
1	D	41	PRO	2.3
1	D	245	THR	2.3
1	D	367	THR	2.3
1	B	43	ALA	2.3
1	A	382	LEU	2.3
1	C	197	GLY	2.3
1	D	359	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	517	LYS	2.3
1	D	83	PHE	2.3
1	A	495	SER	2.3
1	D	260	HIS	2.3
1	D	496	ILE	2.3
1	C	439	PRO	2.3
1	D	443	PRO	2.3
1	C	135	ASN	2.3
1	B	396	LEU	2.3
1	B	539	ASP	2.3
1	C	184	GLY	2.3
1	C	274	GLY	2.3
1	D	418	GLY	2.3
1	C	371	MET	2.3
1	D	271	MET	2.3
1	A	75	HIS	2.3
1	D	293	ILE	2.3
1	A	370	VAL	2.3
1	C	208	THR	2.3
1	C	435	PRO	2.3
1	A	200	ASN	2.3
1	C	151	ARG	2.3
1	A	441	GLY	2.3
1	B	510	LYS	2.3
1	C	20	LYS	2.3
1	C	484	ALA	2.3
1	D	199	ALA	2.3
1	D	318	ALA	2.3
1	D	544	ASP	2.3
1	D	394	LEU	2.3
1	B	370	VAL	2.2
1	B	450[A]	THR	2.2
1	D	310	VAL	2.2
1	D	292	ASN	2.2
1	C	433	ALA	2.2
1	D	485	CYS	2.2
1	C	212	LEU	2.2
1	D	17	LEU	2.2
1	D	110	LEU	2.2
1	D	205	LEU	2.2
1	B	546	PHE	2.2
1	D	508	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	240	VAL	2.2
1	D	238	VAL	2.2
1	B	294	GLY	2.2
1	C	229	GLY	2.2
1	C	453	GLY	2.2
1	D	382	LEU	2.2
1	D	514	LEU	2.2
1	B	164	TYR	2.2
1	D	187	TYR	2.2
1	D	424	TYR	2.2
1	D	168	ASN	2.2
1	D	499	PRO	2.2
1	D	132	VAL	2.2
1	A	448	GLY	2.2
1	C	519	LEU	2.2
1	D	212	LEU	2.2
1	C	37	SER	2.2
1	C	395	SER	2.2
1	C	339	ASN	2.2
1	A	545	PHE	2.1
1	D	308	VAL	2.1
1	D	529	VAL	2.1
1	C	79	LEU	2.1
1	C	396	LEU	2.1
1	C	289	VAL	2.1
1	D	454	ARG	2.1
1	D	265	LEU	2.1
1	D	476	ASN	2.1
1	D	90	ASP	2.1
1	A	269	PRO	2.1
1	C	389	PRO	2.1
1	C	397	THR	2.1
1	D	352	PRO	2.1
1	C	260	HIS	2.1
1	A	124	GLY	2.1
1	C	147	ILE	2.1
1	D	54	ALA	2.1
1	C	161	LEU	2.1
1	A	378	MET	2.1
1	C	160	PRO	2.1
1	A	118	GLY	2.1
1	C	288	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	215	LYS	2.1
1	A	478	SER	2.1
1	C	247	ALA	2.1
1	D	504	ALA	2.1
1	C	280	LEU	2.0
1	D	111	LEU	2.0
1	B	152	ASN	2.0
1	C	178	ASP	2.0
1	D	320	CYS	2.0
1	D	150	LYS	2.0
1	C	434	GLY	2.0
1	D	520	GLY	2.0
1	C	257	ALA	2.0
1	D	63	ALA	2.0
1	D	387	LYS	2.0
1	B	304	TYR	2.0
1	C	256	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	606	6/6	0.90	0.18	26,28,30,34	0
3	GOL	A	605	6/6	0.91	0.16	26,31,34,34	0
3	GOL	A	604	6/6	0.92	0.13	27,33,37,38	0
3	GOL	B	603	6/6	0.93	0.10	22,25,26,27	0
5	JYD	B	604[A]	9/9	0.93	0.14	9,11,13,16	9
5	JYD	B	604[B]	9/9	0.93	0.14	9,10,12,14	9

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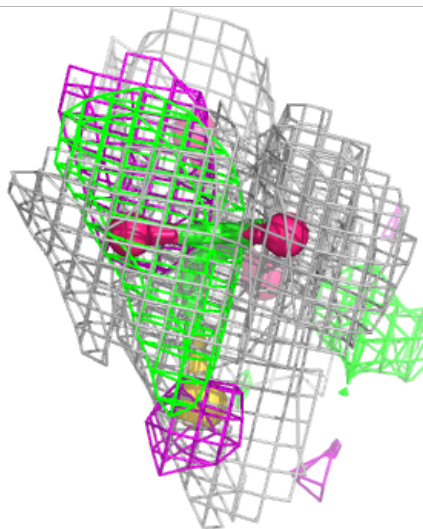
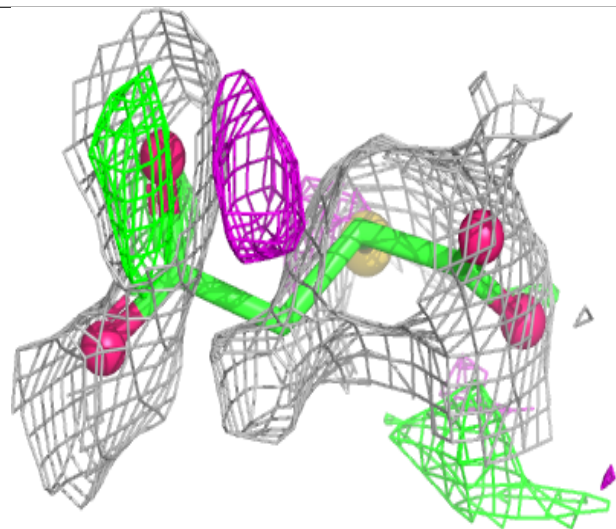
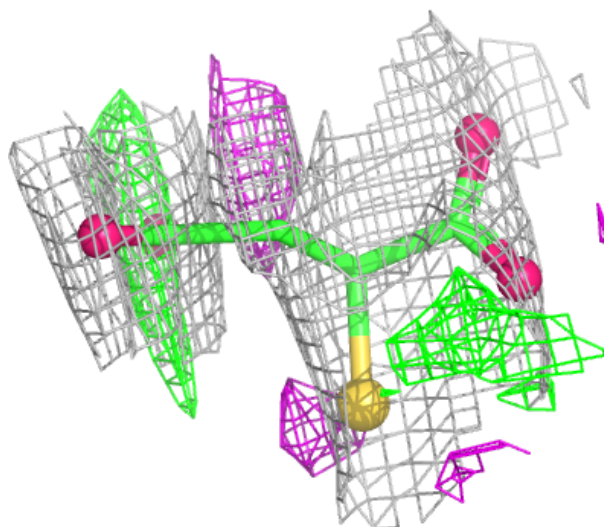
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	JYD	C	604	9/9	0.94	0.17	30,35,42,45	0
5	JYD	D	602	9/9	0.94	0.13	22,32,34,36	0
4	1PE	A	610	10/16	0.95	0.10	10,29,36,39	0
4	1PE	B	606	10/16	0.96	0.10	24,35,37,37	0
4	1PE	C	605	10/16	0.96	0.11	30,37,41,42	0
4	1PE	C	606	10/16	0.96	0.09	26,32,35,35	0
4	1PE	D	603	16/16	0.96	0.12	26,32,35,35	0
3	GOL	C	602	6/6	0.96	0.13	40,42,43,43	0
4	1PE	A	607	7/16	0.96	0.11	28,29,32,36	0
4	1PE	A	609	13/16	0.96	0.08	14,21,27,30	0
3	GOL	A	603	6/6	0.96	0.07	24,26,32,34	0
5	JYD	A	608[B]	9/9	0.97	0.10	16,17,18,18	9
4	1PE	B	605	13/16	0.97	0.09	15,17,23,24	0
3	GOL	A	602	6/6	0.97	0.08	21,25,29,31	0
4	1PE	C	603	7/16	0.97	0.08	27,28,30,31	0
5	JYD	A	608[A]	9/9	0.97	0.10	17,17,18,21	9
3	GOL	B	602	6/6	0.98	0.08	26,27,29,30	0
2	SF4	D	601	8/8	0.98	0.10	23,32,34,39	0
2	SF4	C	601	8/8	0.98	0.09	24,30,31,31	0
4	1PE	A	611	10/16	0.98	0.09	29,31,34,34	0
2	SF4	A	601	8/8	0.99	0.06	15,19,22,22	0
2	SF4	B	601	8/8	0.99	0.07	14,21,23,24	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.

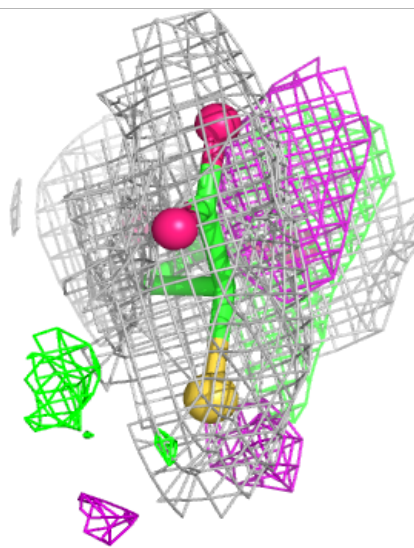
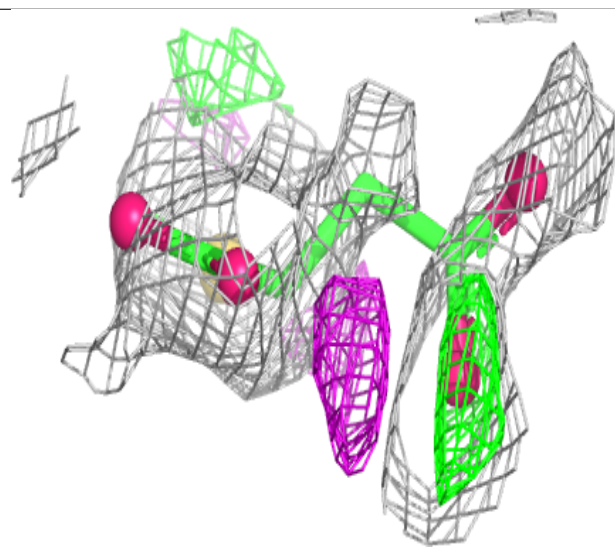
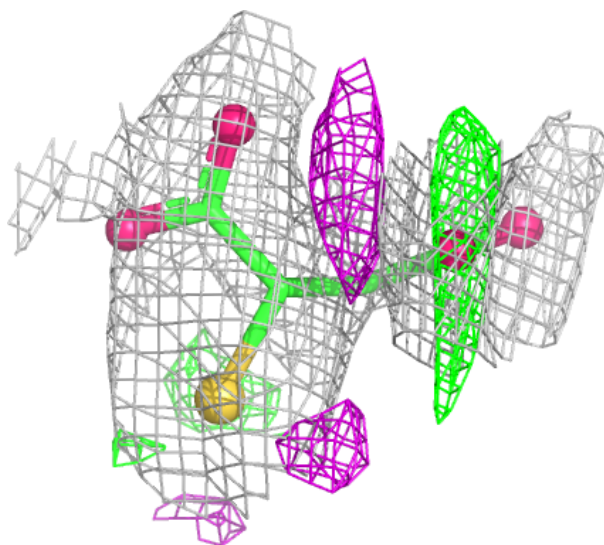
Electron density around JYD B 604 (A):

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



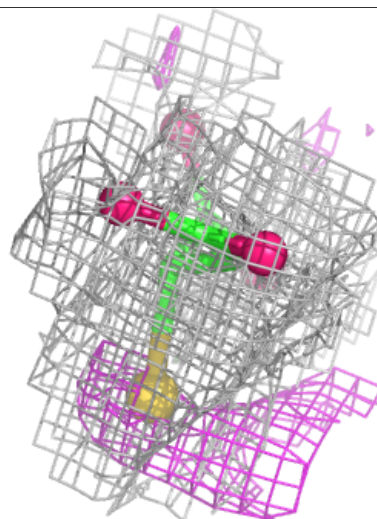
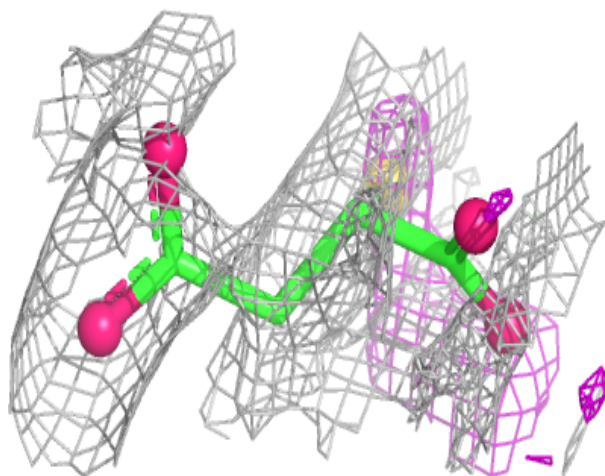
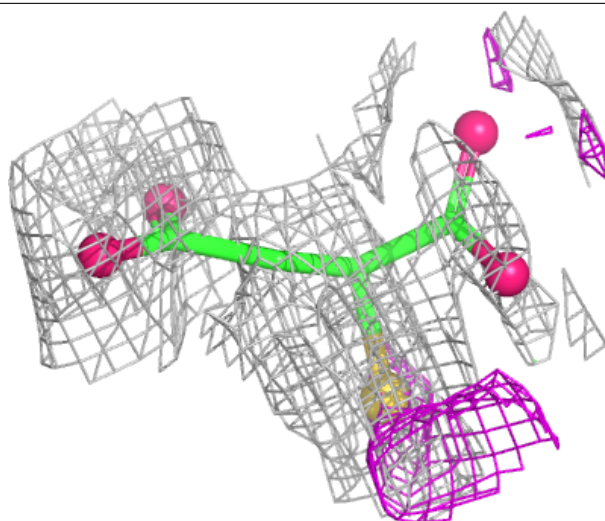
Electron density around JYD B 604 (B):

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



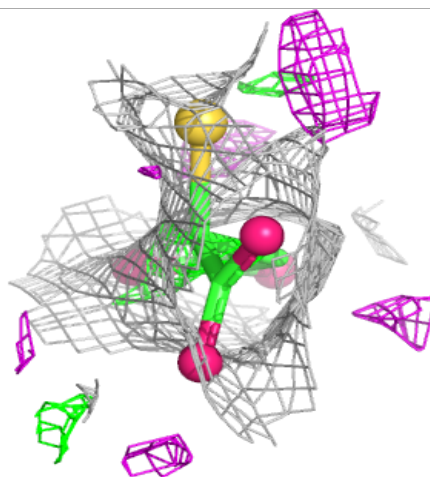
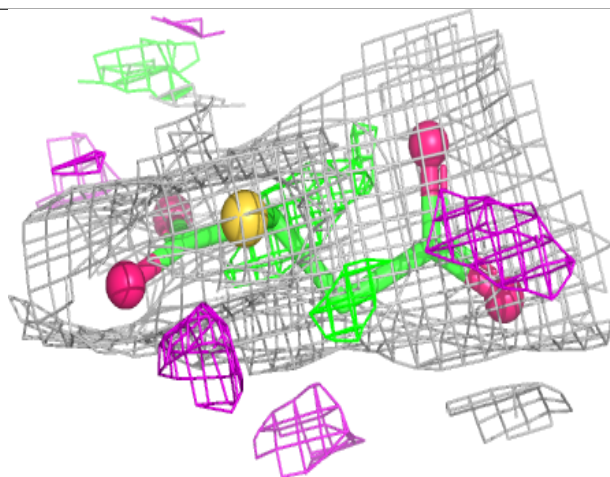
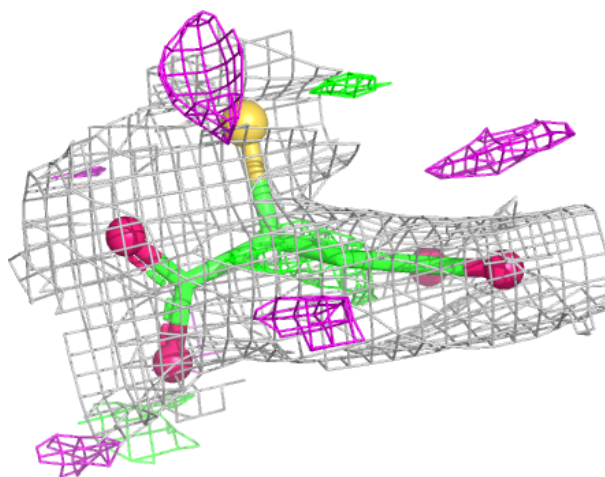
Electron density around JYD C 604:

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



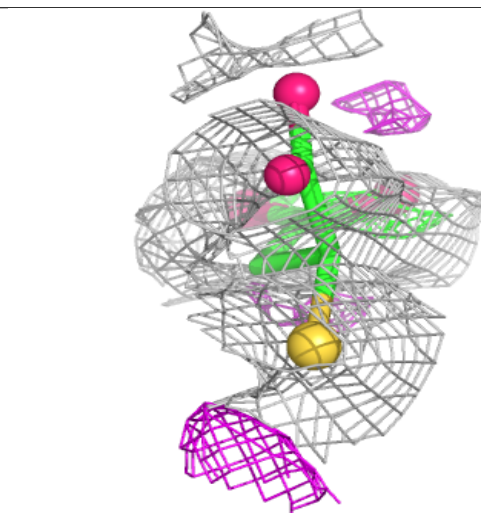
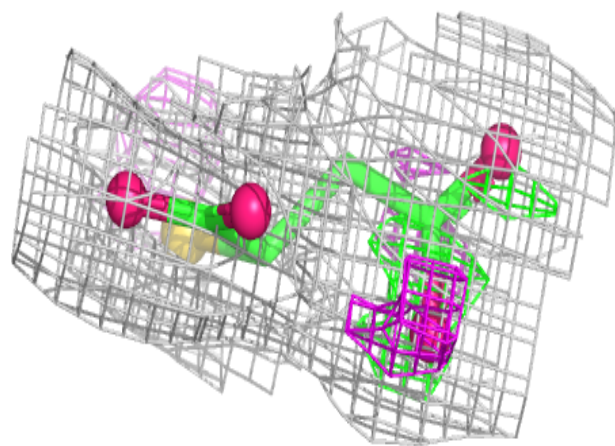
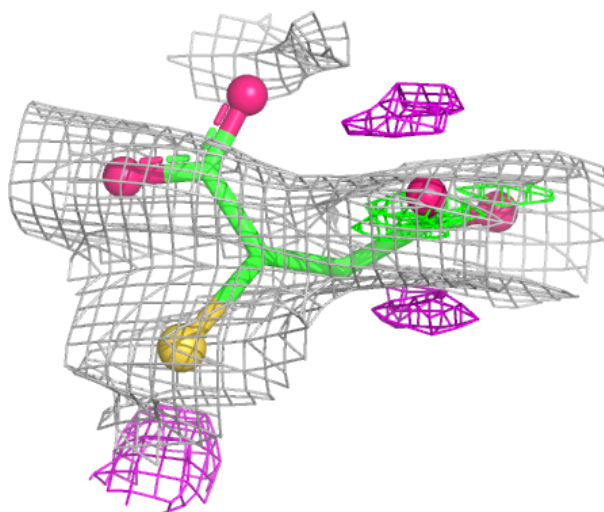
Electron density around JYD D 602:

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



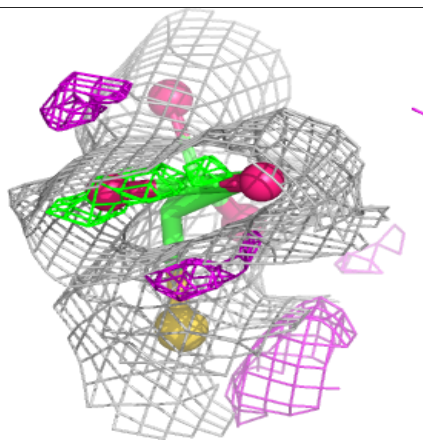
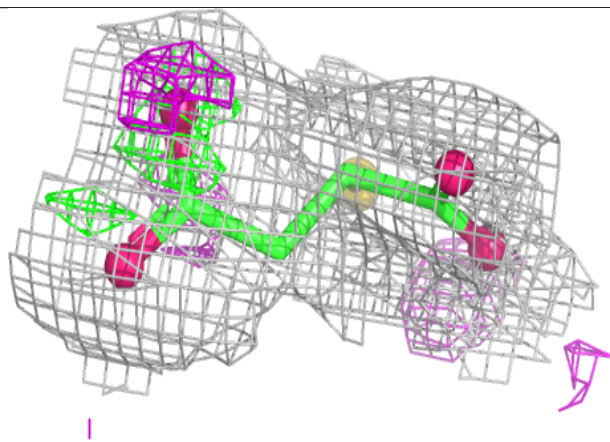
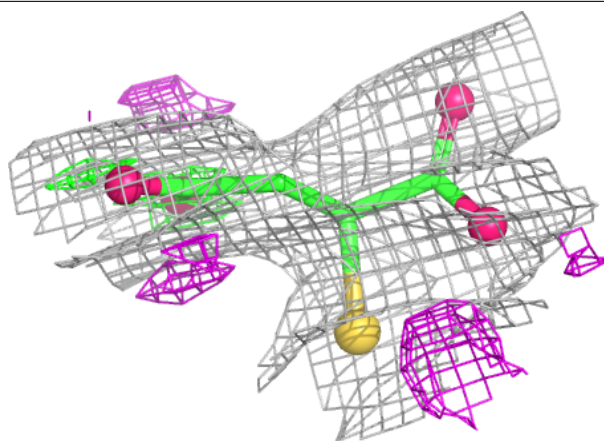
Electron density around JYD A 608 (B):

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.