



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 07:55 PM UTC

PDB ID : 4L9Y / pdb_00004l9y
Title : Crystal Structure of Rhodobacter sphaeroides malyl-CoA lyase in complex with magnesium, glyoxylate, and propionyl-CoA
Authors : Zarzycki, J.; Kerfeld, C.A.
Deposited on : 2013-06-18
Resolution : 2.10 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

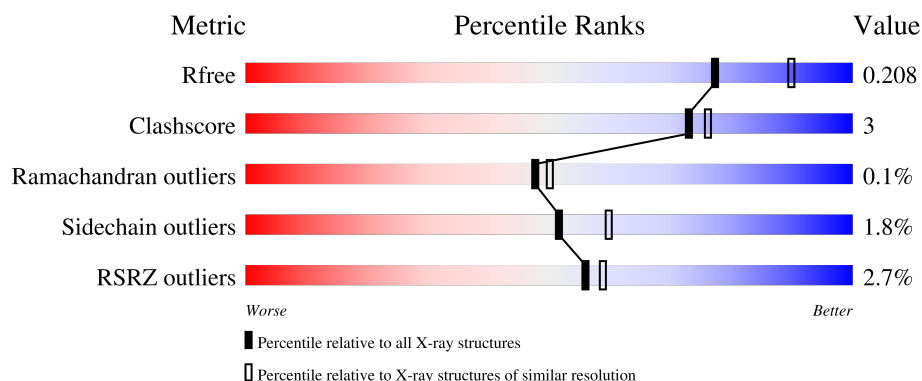
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	339	 2% 86% 6% 7%
1	B	339	 73% 5% 22%
1	C	339	 3% 83% 10% 7%
1	D	339	 71% 7% 22%
1	E	339	 72% 5% 22%

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Mol	Chain	Length	Quality of chain
1	F	339	 7% 83% 8% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14807 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 Malyl-CoA lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2382	1496	425	449	12			
1	B	264	Total	C	N	O	S	0	0	0
			2012	1269	358	375	10			
1	C	316	Total	C	N	O	S	0	0	0
			2396	1505	427	452	12			
1	D	265	Total	C	N	O	S	0	0	0
			2018	1272	359	377	10			
1	E	265	Total	C	N	O	S	0	0	0
			2018	1272	359	377	10			
1	F	309	Total	C	N	O	S	0	0	0
			2340	1472	416	441	11			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q3J5L6
A	-19	GLY	-	expression tag	UNP Q3J5L6
A	-18	HIS	-	expression tag	UNP Q3J5L6
A	-17	HIS	-	expression tag	UNP Q3J5L6
A	-16	HIS	-	expression tag	UNP Q3J5L6
A	-15	HIS	-	expression tag	UNP Q3J5L6
A	-14	HIS	-	expression tag	UNP Q3J5L6
A	-13	HIS	-	expression tag	UNP Q3J5L6
A	-12	HIS	-	expression tag	UNP Q3J5L6
A	-11	HIS	-	expression tag	UNP Q3J5L6
A	-10	HIS	-	expression tag	UNP Q3J5L6
A	-9	HIS	-	expression tag	UNP Q3J5L6
A	-8	SER	-	expression tag	UNP Q3J5L6
A	-7	SER	-	expression tag	UNP Q3J5L6
A	-6	GLY	-	expression tag	UNP Q3J5L6
A	-5	HIS	-	expression tag	UNP Q3J5L6
A	-4	ILE	-	expression tag	UNP Q3J5L6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	-	expression tag	UNP Q3J5L6
A	-2	GLY	-	expression tag	UNP Q3J5L6
A	-1	ARG	-	expression tag	UNP Q3J5L6
A	0	HIS	-	expression tag	UNP Q3J5L6
B	-20	MET	-	expression tag	UNP Q3J5L6
B	-19	GLY	-	expression tag	UNP Q3J5L6
B	-18	HIS	-	expression tag	UNP Q3J5L6
B	-17	HIS	-	expression tag	UNP Q3J5L6
B	-16	HIS	-	expression tag	UNP Q3J5L6
B	-15	HIS	-	expression tag	UNP Q3J5L6
B	-14	HIS	-	expression tag	UNP Q3J5L6
B	-13	HIS	-	expression tag	UNP Q3J5L6
B	-12	HIS	-	expression tag	UNP Q3J5L6
B	-11	HIS	-	expression tag	UNP Q3J5L6
B	-10	HIS	-	expression tag	UNP Q3J5L6
B	-9	HIS	-	expression tag	UNP Q3J5L6
B	-8	SER	-	expression tag	UNP Q3J5L6
B	-7	SER	-	expression tag	UNP Q3J5L6
B	-6	GLY	-	expression tag	UNP Q3J5L6
B	-5	HIS	-	expression tag	UNP Q3J5L6
B	-4	ILE	-	expression tag	UNP Q3J5L6
B	-3	GLU	-	expression tag	UNP Q3J5L6
B	-2	GLY	-	expression tag	UNP Q3J5L6
B	-1	ARG	-	expression tag	UNP Q3J5L6
B	0	HIS	-	expression tag	UNP Q3J5L6
C	-20	MET	-	expression tag	UNP Q3J5L6
C	-19	GLY	-	expression tag	UNP Q3J5L6
C	-18	HIS	-	expression tag	UNP Q3J5L6
C	-17	HIS	-	expression tag	UNP Q3J5L6
C	-16	HIS	-	expression tag	UNP Q3J5L6
C	-15	HIS	-	expression tag	UNP Q3J5L6
C	-14	HIS	-	expression tag	UNP Q3J5L6
C	-13	HIS	-	expression tag	UNP Q3J5L6
C	-12	HIS	-	expression tag	UNP Q3J5L6
C	-11	HIS	-	expression tag	UNP Q3J5L6
C	-10	HIS	-	expression tag	UNP Q3J5L6
C	-9	HIS	-	expression tag	UNP Q3J5L6
C	-8	SER	-	expression tag	UNP Q3J5L6
C	-7	SER	-	expression tag	UNP Q3J5L6
C	-6	GLY	-	expression tag	UNP Q3J5L6
C	-5	HIS	-	expression tag	UNP Q3J5L6
C	-4	ILE	-	expression tag	UNP Q3J5L6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLU	-	expression tag	UNP Q3J5L6
C	-2	GLY	-	expression tag	UNP Q3J5L6
C	-1	ARG	-	expression tag	UNP Q3J5L6
C	0	HIS	-	expression tag	UNP Q3J5L6
D	-20	MET	-	expression tag	UNP Q3J5L6
D	-19	GLY	-	expression tag	UNP Q3J5L6
D	-18	HIS	-	expression tag	UNP Q3J5L6
D	-17	HIS	-	expression tag	UNP Q3J5L6
D	-16	HIS	-	expression tag	UNP Q3J5L6
D	-15	HIS	-	expression tag	UNP Q3J5L6
D	-14	HIS	-	expression tag	UNP Q3J5L6
D	-13	HIS	-	expression tag	UNP Q3J5L6
D	-12	HIS	-	expression tag	UNP Q3J5L6
D	-11	HIS	-	expression tag	UNP Q3J5L6
D	-10	HIS	-	expression tag	UNP Q3J5L6
D	-9	HIS	-	expression tag	UNP Q3J5L6
D	-8	SER	-	expression tag	UNP Q3J5L6
D	-7	SER	-	expression tag	UNP Q3J5L6
D	-6	GLY	-	expression tag	UNP Q3J5L6
D	-5	HIS	-	expression tag	UNP Q3J5L6
D	-4	ILE	-	expression tag	UNP Q3J5L6
D	-3	GLU	-	expression tag	UNP Q3J5L6
D	-2	GLY	-	expression tag	UNP Q3J5L6
D	-1	ARG	-	expression tag	UNP Q3J5L6
D	0	HIS	-	expression tag	UNP Q3J5L6
E	-20	MET	-	expression tag	UNP Q3J5L6
E	-19	GLY	-	expression tag	UNP Q3J5L6
E	-18	HIS	-	expression tag	UNP Q3J5L6
E	-17	HIS	-	expression tag	UNP Q3J5L6
E	-16	HIS	-	expression tag	UNP Q3J5L6
E	-15	HIS	-	expression tag	UNP Q3J5L6
E	-14	HIS	-	expression tag	UNP Q3J5L6
E	-13	HIS	-	expression tag	UNP Q3J5L6
E	-12	HIS	-	expression tag	UNP Q3J5L6
E	-11	HIS	-	expression tag	UNP Q3J5L6
E	-10	HIS	-	expression tag	UNP Q3J5L6
E	-9	HIS	-	expression tag	UNP Q3J5L6
E	-8	SER	-	expression tag	UNP Q3J5L6
E	-7	SER	-	expression tag	UNP Q3J5L6
E	-6	GLY	-	expression tag	UNP Q3J5L6
E	-5	HIS	-	expression tag	UNP Q3J5L6
E	-4	ILE	-	expression tag	UNP Q3J5L6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLU	-	expression tag	UNP Q3J5L6
E	-2	GLY	-	expression tag	UNP Q3J5L6
E	-1	ARG	-	expression tag	UNP Q3J5L6
E	0	HIS	-	expression tag	UNP Q3J5L6
F	-20	MET	-	expression tag	UNP Q3J5L6
F	-19	GLY	-	expression tag	UNP Q3J5L6
F	-18	HIS	-	expression tag	UNP Q3J5L6
F	-17	HIS	-	expression tag	UNP Q3J5L6
F	-16	HIS	-	expression tag	UNP Q3J5L6
F	-15	HIS	-	expression tag	UNP Q3J5L6
F	-14	HIS	-	expression tag	UNP Q3J5L6
F	-13	HIS	-	expression tag	UNP Q3J5L6
F	-12	HIS	-	expression tag	UNP Q3J5L6
F	-11	HIS	-	expression tag	UNP Q3J5L6
F	-10	HIS	-	expression tag	UNP Q3J5L6
F	-9	HIS	-	expression tag	UNP Q3J5L6
F	-8	SER	-	expression tag	UNP Q3J5L6
F	-7	SER	-	expression tag	UNP Q3J5L6
F	-6	GLY	-	expression tag	UNP Q3J5L6
F	-5	HIS	-	expression tag	UNP Q3J5L6
F	-4	ILE	-	expression tag	UNP Q3J5L6
F	-3	GLU	-	expression tag	UNP Q3J5L6
F	-2	GLY	-	expression tag	UNP Q3J5L6
F	-1	ARG	-	expression tag	UNP Q3J5L6
F	0	HIS	-	expression tag	UNP Q3J5L6

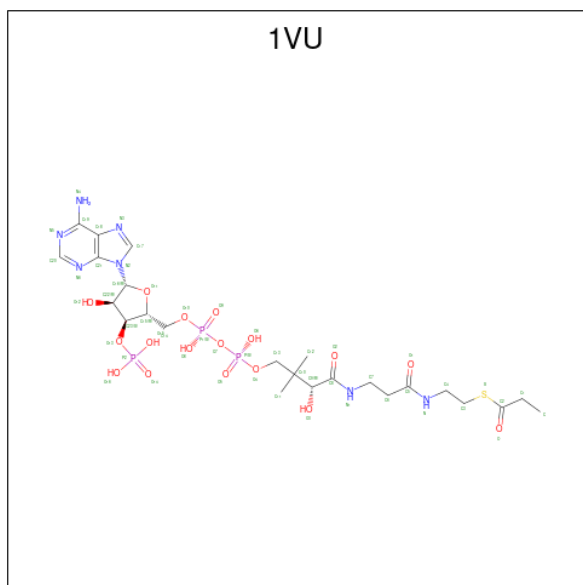
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

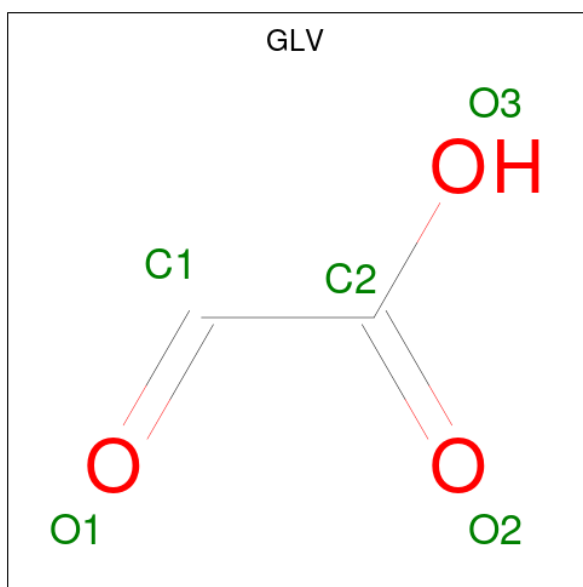
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is propionyl Coenzyme A (CCD ID: 1VU) (formula: $C_{24}H_{40}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		

- Molecule 5 is GLYOXYLIC ACID (CCD ID: GLV) (formula: $C_2H_2O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			5	2	3		
5	D	1	Total	C	O	0	0
			5	2	3		

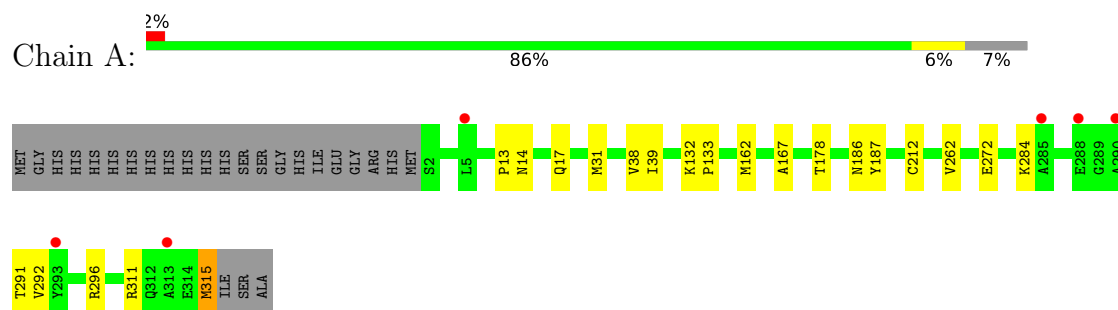
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total	O	0	0
			210	210		
6	B	244	Total	O	0	0
			244	244		
6	C	308	Total	O	0	0
			308	308		
6	D	261	Total	O	0	0
			261	261		
6	E	260	Total	O	0	0
			260	260		
6	F	286	Total	O	0	0
			286	286		

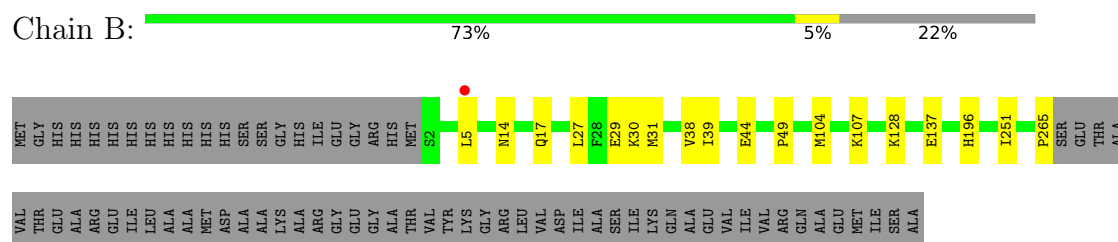
3 Residue-property plots

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.

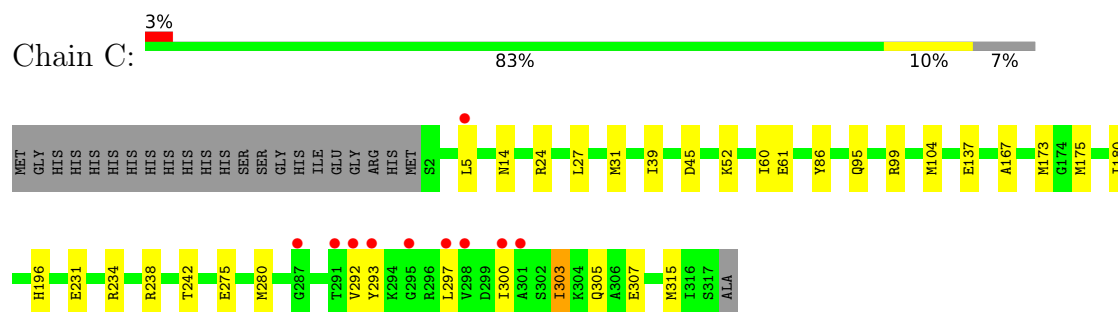
• Molecule 1: Maly-CoA lyase



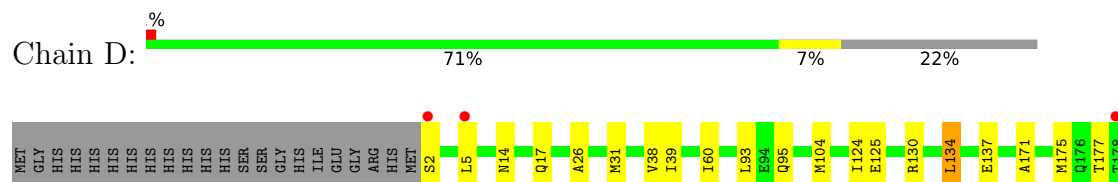
• Molecule 1: Maly-CoA lyase



• Molecule 1: Maly-CoA lyase



• Molecule 1: Maly-CoA lyase





MET	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	HIS	TLE	GLU	GLY	ARG	HIS	MET	S2	F3	R4	L5	O6	M14	K30	N31	A32	I39	K71	E94	M104	K128	E137	A167	I180	M196	D230	T242	H252	P263	K254								
	THR	ALA	VAL	THR	GLU	ALA	ARG	GLU	ILE	LEU	ALA	ALA	ALA	LYS	LYS	ALA	ASP	ILE	ALA	GLY	GLU	ALA	THR	VAL	TYR	LYS	ARG	LEU	VAL	ASP	ILE	ALA	SER	ILE	LYS	GLN	ALA	GLU	VAL	ILE	VAL	ARG	GLN	ALA	GLU	MET	ILE	SER	ALA

- Molecule 1: Malyl-CoA lyase

	W249	MET
	P265 ●	GLY
	S266 ●	HIS
	E267	HIS
	T268	HIS
	A269 ●	HIS
	V270	HIS
	T271	HIS
	E272	HIS
	L276 ●	HIS
	L277	SER
	A278	SER
	A279 ●	GLY
	M280	ILE
	D281	ILE
	A282 ●	GLU
	A283	GLY
	G287 ●	ARG
	G289 ●	HIS
	A290	MET
	T291 ●	\$2
	V292 ●	\$5
	L297 ●	N14
	V298 ●	M31
	D299 ●	S34
	A300	I39
	A301 ●	E44
	S302	K71
	I303 ●	Q95
	K304	R126
	Q305	A154
	A306 ●	A167
	E307	I180
	V308	Y187
	I309 ●	D192
	V310	H215
	ARG	P223
	GLN	D230
	ALA	
	GLU	
	MET	
	ILE	
	SER	
	ALA	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.21Å 144.00Å 94.22Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	38.79 – 2.10 38.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.79-2.10) 99.4 (38.79-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.2_1303	Depositor
R, R_{free}	0.177 , 0.207 0.178 , 0.208	Depositor DCC
R_{free} test set	1995 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14807	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLV, MG, CL, 1VU

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	0.29	0/2431	0.72	0/3300
1	B	0.30	0/2060	0.72	0/2801
1	C	0.31	0/2445	0.70	0/3319
1	D	0.31	0/2066	0.72	0/2809
1	E	0.31	0/2066	0.73	1/2809 (0.0%)
1	F	0.31	0/2389	0.71	0/3245
All	All	0.31	0/13457	0.72	1/18283 (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	E	4	ARG	N-CA-C	-5.31	101.29	109.52

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	2382	0	2350	14	0
1	B	2012	0	1966	13	0
1	C	2396	0	2366	20	0
1	D	2018	0	1971	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2018	0	1971	15	0
1	F	2340	0	2309	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	1	0
3	C	1	0	0	0	0
3	E	1	0	0	1	0
3	F	1	0	0	0	0
4	B	52	0	38	1	0
5	B	5	0	1	0	0
5	D	5	0	1	0	0
6	A	210	0	0	3	0
6	B	244	0	0	2	0
6	C	308	0	0	4	0
6	D	261	0	0	4	0
6	E	260	0	0	4	1
6	F	286	0	0	3	1
All	All	14807	0	12973	83	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (83) 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:178:THR:O	6:A:700:HOH:O	1.91	0.86
1:A:262:VAL:O	6:A:618:HOH:O	1.93	0.83
1:C:61:GLU:OE1	6:C:786:HOH:O	2.00	0.79
1:D:26:ALA:O	6:D:630:HOH:O	2.04	0.76
1:E:4:ARG:NH1	6:E:742:HOH:O	2.20	0.74
1:E:32:ALA:O	6:E:619:HOH:O	2.08	0.70
1:E:230:ASP:OD2	6:E:684:HOH:O	2.13	0.67
1:B:265:PRO:O	6:B:681:HOH:O	2.12	0.67
1:D:2:SER:O	6:D:675:HOH:O	2.12	0.67
1:F:230:ASP:OD2	6:F:707:HOH:O	2.16	0.61
1:E:94:GLU:HG2	1:E:128:LYS:HE3	1.85	0.59
1:D:231:GLU:OE1	6:D:600:HOH:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:ALA:HB2	1:F:180:ILE:HG23	1.87	0.56
1:E:30:LYS:NZ	6:E:756:HOH:O	2.39	0.56
1:F:34:SER:O	1:F:71:LYS:NZ	2.29	0.56
1:C:31:MET:HE2	1:C:39:ILE:HG23	1.86	0.55
1:C:231:GLU:OE2	1:C:234:ARG:NH1	2.40	0.54
1:E:167:ALA:HB2	1:E:180:ILE:HG23	1.89	0.54
1:A:17:GLN:HG2	1:A:38:VAL:HB	1.91	0.53
1:B:44:GLU:OE2	1:B:107:LYS:NZ	2.37	0.52
1:C:167:ALA:HB2	1:C:180:ILE:HG23	1.92	0.52
1:C:275:GLU:OE1	1:C:293:TYR:OH	2.25	0.51
1:A:272:GLU:OE2	1:A:296:ARG:NH1	2.44	0.51
1:A:284:LYS:HZ3	1:B:49:PRO:HD2	1.77	0.50
1:F:307:GLU:HA	1:F:310:VAL:HG22	1.94	0.50
1:F:223:PRO:HD3	1:F:249:TRP:CE3	2.47	0.49
1:F:126:ARG:HG3	6:F:667:HOH:O	2.11	0.49
1:D:175:MET:HB3	1:D:177:THR:HG23	1.95	0.48
1:A:31:MET:HE2	1:A:39:ILE:HG23	1.96	0.48
1:F:287:GLY:HA2	6:F:719:HOH:O	2.14	0.47
1:B:30:LYS:NZ	4:B:401:1VU:O12	2.39	0.47
1:E:31:MET:HE2	1:E:39:ILE:HG23	1.96	0.47
1:F:270:VAL:HG23	1:F:310:VAL:HG12	1.95	0.47
1:F:60:ILE:HD13	1:F:95:GLN:HB2	1.95	0.47
1:E:104:MET:HE3	1:E:137:GLU:CD	2.40	0.47
1:D:31:MET:HE2	1:D:39:ILE:HG23	1.96	0.46
1:C:52:LYS:HB3	6:C:581:HOH:O	2.16	0.46
1:E:5:LEU:HB3	1:E:6:GLN:H	1.55	0.46
1:F:267:GLU:HA	1:F:270:VAL:HG12	1.97	0.46
1:C:280:MET:SD	1:C:303:ILE:HD12	2.55	0.46
1:A:13:PRO:HA	1:A:315:MET:HE3	1.97	0.46
1:B:31:MET:HE2	1:B:39:ILE:HG23	1.98	0.45
1:B:196:HIS:CD2	1:C:196:HIS:HD2	2.35	0.45
1:B:29:GLU:HB2	6:B:614:HOH:O	2.15	0.45
1:C:45:ASP:OD2	6:C:503:HOH:O	2.21	0.44
1:D:252:HIS:ND1	1:D:254:LYS:HG2	2.33	0.44
1:D:17:GLN:HG2	1:D:38:VAL:HB	2.00	0.44
1:F:31:MET:HE2	1:F:39:ILE:HG23	2.00	0.43
1:D:93:LEU:HD11	1:D:134:LEU:HD22	2.01	0.43
1:E:128:LYS:HA	1:E:128:LYS:HD3	1.88	0.43
1:A:132:LYS:HA	1:A:133:PRO:HD2	1.91	0.43
1:D:125:GLU:HG2	1:D:130:ARG:HD3	2.01	0.43
1:D:177:THR:O	6:D:591:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ALA:HB3	3:A:402:CL:CL	2.56	0.42
1:D:104:MET:HE3	1:D:137:GLU:CD	2.45	0.42
1:D:238:ARG:HB3	1:E:186:ASN:HB3	2.00	0.42
1:B:27:LEU:O	1:B:31:MET:HG3	2.19	0.42
1:A:162:MET:HB3	1:A:212:CYS:SG	2.60	0.42
1:E:242:THR:HG21	1:F:187:TYR:HB2	2.01	0.41
1:E:167:ALA:HB3	3:E:402:CL:CL	2.57	0.41
1:C:86:TYR:CZ	1:D:124:ILE:HG12	2.55	0.41
1:C:280:MET:HE2	1:C:280:MET:HB3	2.00	0.41
1:F:154:ALA:HB2	1:F:215:HIS:CE1	2.56	0.41
1:F:280:MET:HB3	1:F:280:MET:HE3	1.72	0.41
1:B:17:GLN:HG2	1:B:38:VAL:HB	2.01	0.41
1:C:60:ILE:HD13	1:C:95:GLN:HB2	2.03	0.41
1:C:104:MET:HE3	1:C:137:GLU:CD	2.46	0.41
1:C:305:GLN:OE1	6:C:772:HOH:O	2.22	0.41
1:E:32:ALA:O	1:E:71:LYS:HE2	2.21	0.41
1:B:104:MET:HE3	1:B:137:GLU:CD	2.44	0.41
1:E:252:HIS:ND1	1:E:254:LYS:HG2	2.35	0.41
1:A:186:ASN:HB3	1:C:238:ARG:HB3	2.03	0.41
1:A:291:THR:OG1	1:A:292:VAL:N	2.54	0.41
1:A:311:ARG:O	6:A:696:HOH:O	2.22	0.41
1:B:251:ILE:H	1:B:251:ILE:HG13	1.77	0.41
1:C:24:ARG:CZ	1:C:27:LEU:HD11	2.51	0.41
1:D:60:ILE:HD13	1:D:95:GLN:HB2	2.03	0.41
1:A:187:TYR:HB2	1:C:242:THR:HG21	2.02	0.41
1:B:196:HIS:HD2	1:C:196:HIS:HD2	1.68	0.40
1:B:128:LYS:HA	1:B:128:LYS:HD3	1.92	0.40
1:C:99:ARG:HA	1:C:99:ARG:HD2	1.88	0.40
1:C:173:MET:HB2	1:C:175:MET:HG3	2.03	0.40
1:D:171:ALA:HB2	1:F:305:GLN:HG3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:568:HOH:O	6:F:534:HOH:O[2_556]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/339 (92%)	306 (98%)	6 (2%)	0	100	100
1	B	262/339 (77%)	256 (98%)	6 (2%)	0	100	100
1	C	314/339 (93%)	306 (98%)	8 (2%)	0	100	100
1	D	263/339 (78%)	257 (98%)	6 (2%)	0	100	100
1	E	263/339 (78%)	256 (97%)	6 (2%)	1 (0%)	30	28
1	F	307/339 (91%)	299 (97%)	7 (2%)	1 (0%)	36	36
All	All	1721/2034 (85%)	1680 (98%)	39 (2%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	5	LEU
1	F	192	ASP

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	239/260 (92%)	237 (99%)	2 (1%)	73	81
1	B	203/260 (78%)	201 (99%)	2 (1%)	68	76
1	C	241/260 (93%)	233 (97%)	8 (3%)	33	37
1	D	204/260 (78%)	200 (98%)	4 (2%)	48	56
1	E	204/260 (78%)	201 (98%)	3 (2%)	57	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	235/260 (90%)	230 (98%)	5 (2%)	47 54
All	All	1326/1560 (85%)	1302 (98%)	24 (2%)	51 60

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	315	MET
1	B	5	LEU
1	B	14	ASN
1	C	5	LEU
1	C	14	ASN
1	C	292	VAL
1	C	297	LEU
1	C	300	ILE
1	C	303	ILE
1	C	307	GLU
1	C	315	MET
1	D	5	LEU
1	D	14	ASN
1	D	134	LEU
1	D	251	ILE
1	E	4	ARG
1	E	5	LEU
1	E	14	ASN
1	F	14	ASN
1	F	44	GLU
1	F	272	GLU
1	F	297	LEU
1	F	298	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	102	GLN
1	A	305	GLN
1	A	312	GLN
1	B	54	GLN
1	B	196	HIS
1	C	54	GLN

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Mol	Chain	Res	Type
1	C	176	GLN
1	C	186	ASN
1	C	196	HIS
1	C	305	GLN
1	D	176	GLN
1	D	196	HIS
1	E	196	HIS
1	F	54	GLN
1	F	194	GLN
1	F	196	HIS
1	F	215	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 10 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GLV	D	401	2	4,4,4	1.38	0	3,4,4	1.46	0
5	GLV	B	402	2	4,4,4	1.37	0	3,4,4	1.45	0
4	1VU	B	401	-	52,54,54	1.44	8 (15%)	73,80,80	1.82	16 (21%)

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
5	GLV	D	401	2	-	0/0/2/2	-
5	GLV	B	402	2	-	0/0/2/2	-
4	1VU	B	401	-	-	9/53/69/69	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	1VU	C2-S	-4.29	1.66	1.76
4	B	401	1VU	C21-N2	-3.14	1.31	1.37
4	B	401	1VU	C17-N2	-2.90	1.32	1.37
4	B	401	1VU	C18-N3	-2.73	1.34	1.39
4	B	401	1VU	P1-O8	-2.49	1.43	1.55
4	B	401	1VU	P2-O14	-2.19	1.43	1.50
4	B	401	1VU	P-O5	-2.11	1.43	1.50
4	B	401	1VU	O-C2	-2.07	1.17	1.21

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	1VU	C1-C2-S	7.60	123.14	113.56
4	B	401	1VU	C18-C21-N6	-4.80	120.11	126.72
4	B	401	1VU	N5-C20-N6	-3.71	122.97	128.58
4	B	401	1VU	O-C2-C1	-3.63	118.28	123.72
4	B	401	1VU	C21-C18-N3	-3.45	106.64	110.58
4	B	401	1VU	N2-C17-N3	-3.43	109.07	113.94
4	B	401	1VU	O-C2-S	-3.23	118.58	122.68
4	B	401	1VU	C20-N6-C21	2.89	118.88	111.83
4	B	401	1VU	N6-C21-N2	2.80	131.92	127.17
4	B	401	1VU	C21-N2-C17	2.73	108.61	105.74
4	B	401	1VU	C18-N3-C17	2.72	107.73	103.45
4	B	401	1VU	O12-C22-C23	-2.51	104.17	111.19
4	B	401	1VU	O13-C23-C22	-2.38	103.14	111.68
4	B	401	1VU	O10-P1-O9	2.36	118.29	108.94
4	B	401	1VU	C3-S-C2	2.09	108.03	101.84
4	B	401	1VU	C11-C10-C13	2.03	111.57	108.22

There are no chirality outliers.

All (9) torsion outliers are listed below:

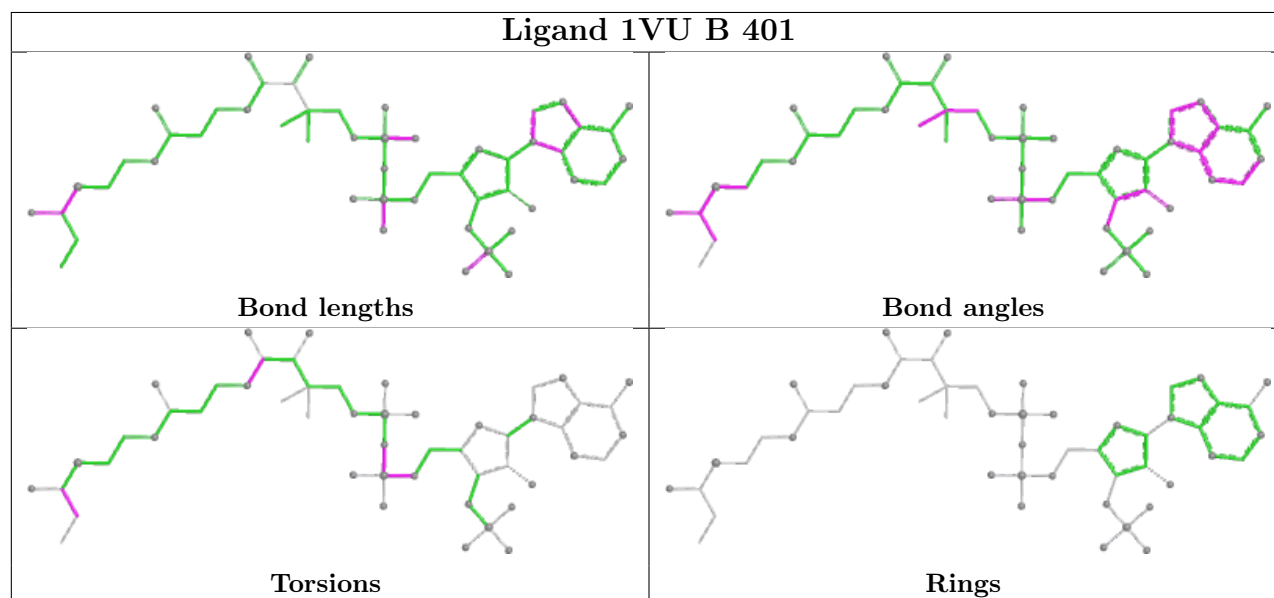
Mol	Chain	Res	Type	Atoms
4	B	401	1VU	C14-O10-P1-O8
4	B	401	1VU	C14-O10-P1-O9
4	B	401	1VU	C14-O10-P1-O7
4	B	401	1VU	C-C1-C2-S
4	B	401	1VU	C-C1-C2-O
4	B	401	1VU	C9-C8-N1-C7
4	B	401	1VU	O2-C8-N1-C7
4	B	401	1VU	P-O7-P1-O8
4	B	401	1VU	P-O7-P1-O9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	1VU	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.



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	314/339 (92%)	0.02	6 (1%) 66 69	12, 26, 52, 62	0
1	B	264/339 (77%)	-0.33	1 (0%) 88 90	11, 21, 36, 43	0
1	C	316/339 (93%)	-0.18	10 (3%) 50 53	9, 19, 52, 77	0
1	D	265/339 (78%)	-0.47	5 (1%) 66 69	8, 17, 34, 52	0
1	E	265/339 (78%)	-0.46	1 (0%) 88 90	8, 17, 31, 53	0
1	F	309/339 (91%)	-0.11	24 (7%) 19 20	8, 17, 57, 65	0
All	All	1733/2034 (85%)	-0.24	47 (2%) 56 59	8, 19, 49, 77	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	301	ALA	5.5
1	C	292	VAL	4.6
1	E	5	LEU	4.1
1	B	5	LEU	4.1
1	F	276	ILE	3.9
1	C	297	LEU	3.9
1	F	287	GLY	3.8
1	F	302	SER	3.3
1	C	295	GLY	3.2
1	C	291	THR	3.2
1	C	298	VAL	3.2
1	F	278	ALA	3.1
1	F	301	ALA	3.0
1	F	297	LEU	3.0
1	C	5	LEU	2.9
1	F	306	ALA	2.9
1	C	287	GLY	2.9
1	F	303	ILE	2.8
1	F	299	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	5	LEU	2.8
1	F	282	ALA	2.7
1	F	266	SER	2.7
1	F	298	VAL	2.7
1	D	2	SER	2.7
1	F	291	THR	2.7
1	D	5	LEU	2.5
1	F	265	PRO	2.4
1	F	279	ALA	2.4
1	F	289	GLY	2.4
1	F	277	LEU	2.3
1	F	309	ILE	2.3
1	F	292	VAL	2.3
1	F	290	ALA	2.3
1	C	300	ILE	2.3
1	C	293	TYR	2.3
1	D	227	PHE	2.2
1	D	266	SER	2.2
1	F	2	SER	2.2
1	A	293	TYR	2.2
1	F	269	ALA	2.2
1	F	283	ALA	2.2
1	F	5	LEU	2.1
1	D	178	THR	2.1
1	A	285	ALA	2.1
1	A	313	ALA	2.1
1	A	288	GLU	2.0
1	A	290	ALA	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,

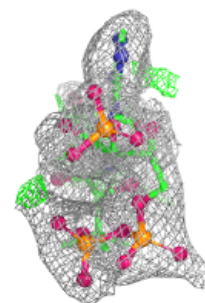
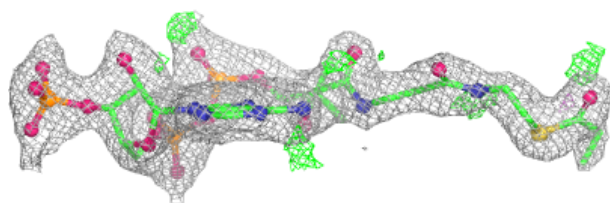
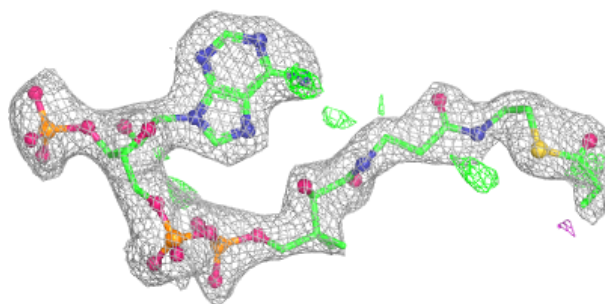
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	1VU	B	401	52/52	0.89	0.10	26,36,44,48	52
5	GLV	B	402	5/5	0.91	0.08	22,23,24,25	5
2	MG	F	401	1/1	0.92	0.04	22,22,22,22	0
2	MG	B	403	1/1	0.94	0.04	26,26,26,26	0
2	MG	D	402	1/1	0.94	0.05	20,20,20,20	0
2	MG	E	401	1/1	0.94	0.05	26,26,26,26	0
5	GLV	D	401	5/5	0.94	0.07	14,16,19,20	5
2	MG	A	401	1/1	0.96	0.04	26,26,26,26	0
2	MG	C	401	1/1	0.96	0.04	21,21,21,21	0
3	CL	A	402	1/1	0.98	0.03	27,27,27,27	0
3	CL	C	402	1/1	0.99	0.06	21,21,21,21	0
3	CL	E	402	1/1	0.99	0.04	21,21,21,21	0
3	CL	F	402	1/1	0.99	0.05	17,17,17,17	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 1VU B 401:

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.