



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2026 – 10:07 AM EDT

PDB ID : 9YQ9 / pdb_00009yq9
Title : Clostridium leptum Carboxyaminopropylagmatine Dehydrogenase Apo
Authors : Ostlund, J.C.; McFarlane, J.S.
Deposited on : 2025-10-15
Resolution : 2.50 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

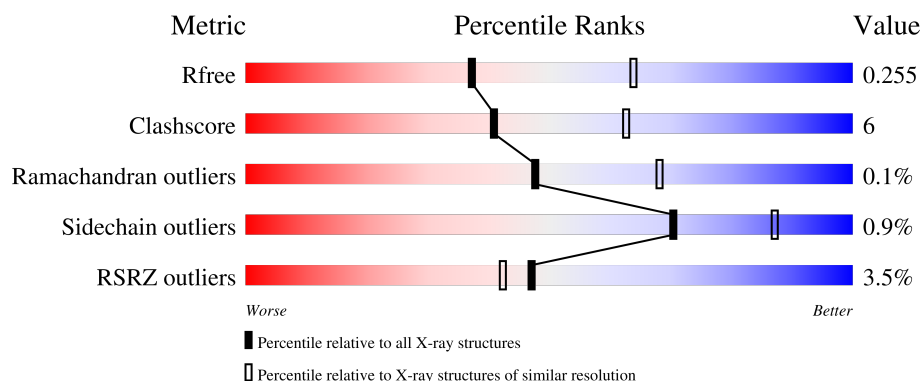
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	417	 3% 73% 13% 13%
1	B	417	 3% 85% 10% 5%
1	C	417	 3% 82% 12% 6%
1	D	417	 3% 72% 11% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21890 atoms, of which 10066 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 Saccharopine dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	361	Total	C	H	N	O	S	0	0	0
			5220	1815	2389	460	535	21			
1	B	397	Total	C	H	N	O	S	0	0	0
			5934	1997	2817	505	593	22			
1	C	391	Total	C	H	N	O	S	0	0	0
			5708	1967	2639	500	580	22			
1	D	350	Total	C	H	N	O	S	0	0	0
			4935	1751	2205	443	515	21			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	HIS	-	expression tag	UNP A7VSG1
A	-16	HIS	-	expression tag	UNP A7VSG1
A	-15	HIS	-	expression tag	UNP A7VSG1
A	-14	HIS	-	expression tag	UNP A7VSG1
A	-13	HIS	-	expression tag	UNP A7VSG1
A	-12	HIS	-	expression tag	UNP A7VSG1
A	-11	SER	-	expression tag	UNP A7VSG1
A	-10	SER	-	expression tag	UNP A7VSG1
A	-9	GLY	-	expression tag	UNP A7VSG1
A	-8	ARG	-	expression tag	UNP A7VSG1
A	-7	GLU	-	expression tag	UNP A7VSG1
A	-6	ASN	-	expression tag	UNP A7VSG1
A	-5	LEU	-	expression tag	UNP A7VSG1
A	-4	TYR	-	expression tag	UNP A7VSG1
A	-3	PHE	-	expression tag	UNP A7VSG1
A	-2	GLN	-	expression tag	UNP A7VSG1
A	-1	GLY	-	expression tag	UNP A7VSG1
A	0	HIS	-	expression tag	UNP A7VSG1
B	-17	HIS	-	expression tag	UNP A7VSG1
B	-16	HIS	-	expression tag	UNP A7VSG1
B	-15	HIS	-	expression tag	UNP A7VSG1

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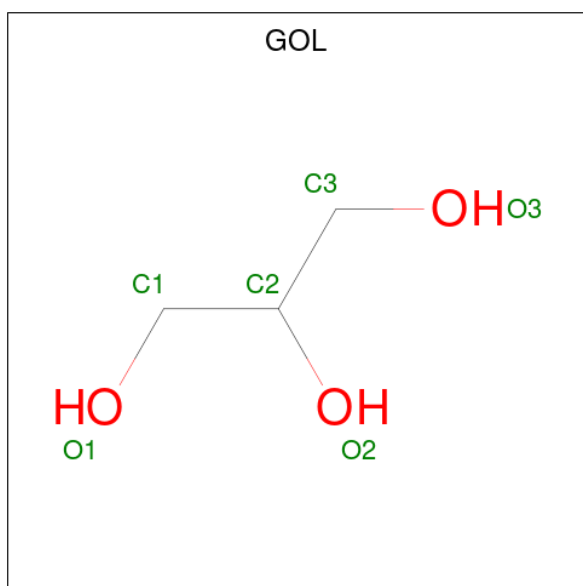
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP A7VSG1
B	-13	HIS	-	expression tag	UNP A7VSG1
B	-12	HIS	-	expression tag	UNP A7VSG1
B	-11	SER	-	expression tag	UNP A7VSG1
B	-10	SER	-	expression tag	UNP A7VSG1
B	-9	GLY	-	expression tag	UNP A7VSG1
B	-8	ARG	-	expression tag	UNP A7VSG1
B	-7	GLU	-	expression tag	UNP A7VSG1
B	-6	ASN	-	expression tag	UNP A7VSG1
B	-5	LEU	-	expression tag	UNP A7VSG1
B	-4	TYR	-	expression tag	UNP A7VSG1
B	-3	PHE	-	expression tag	UNP A7VSG1
B	-2	GLN	-	expression tag	UNP A7VSG1
B	-1	GLY	-	expression tag	UNP A7VSG1
B	0	HIS	-	expression tag	UNP A7VSG1
C	-17	HIS	-	expression tag	UNP A7VSG1
C	-16	HIS	-	expression tag	UNP A7VSG1
C	-15	HIS	-	expression tag	UNP A7VSG1
C	-14	HIS	-	expression tag	UNP A7VSG1
C	-13	HIS	-	expression tag	UNP A7VSG1
C	-12	HIS	-	expression tag	UNP A7VSG1
C	-11	SER	-	expression tag	UNP A7VSG1
C	-10	SER	-	expression tag	UNP A7VSG1
C	-9	GLY	-	expression tag	UNP A7VSG1
C	-8	ARG	-	expression tag	UNP A7VSG1
C	-7	GLU	-	expression tag	UNP A7VSG1
C	-6	ASN	-	expression tag	UNP A7VSG1
C	-5	LEU	-	expression tag	UNP A7VSG1
C	-4	TYR	-	expression tag	UNP A7VSG1
C	-3	PHE	-	expression tag	UNP A7VSG1
C	-2	GLN	-	expression tag	UNP A7VSG1
C	-1	GLY	-	expression tag	UNP A7VSG1
C	0	HIS	-	expression tag	UNP A7VSG1
D	-17	HIS	-	expression tag	UNP A7VSG1
D	-16	HIS	-	expression tag	UNP A7VSG1
D	-15	HIS	-	expression tag	UNP A7VSG1
D	-14	HIS	-	expression tag	UNP A7VSG1
D	-13	HIS	-	expression tag	UNP A7VSG1
D	-12	HIS	-	expression tag	UNP A7VSG1
D	-11	SER	-	expression tag	UNP A7VSG1
D	-10	SER	-	expression tag	UNP A7VSG1
D	-9	GLY	-	expression tag	UNP A7VSG1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	ARG	-	expression tag	UNP A7VSG1
D	-7	GLU	-	expression tag	UNP A7VSG1
D	-6	ASN	-	expression tag	UNP A7VSG1
D	-5	LEU	-	expression tag	UNP A7VSG1
D	-4	TYR	-	expression tag	UNP A7VSG1
D	-3	PHE	-	expression tag	UNP A7VSG1
D	-2	GLN	-	expression tag	UNP A7VSG1
D	-1	GLY	-	expression tag	UNP A7VSG1
D	0	HIS	-	expression tag	UNP A7VSG1

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	28	Total	O	0	0
			28	28		
3	C	26	Total	O	0	0
			26	26		

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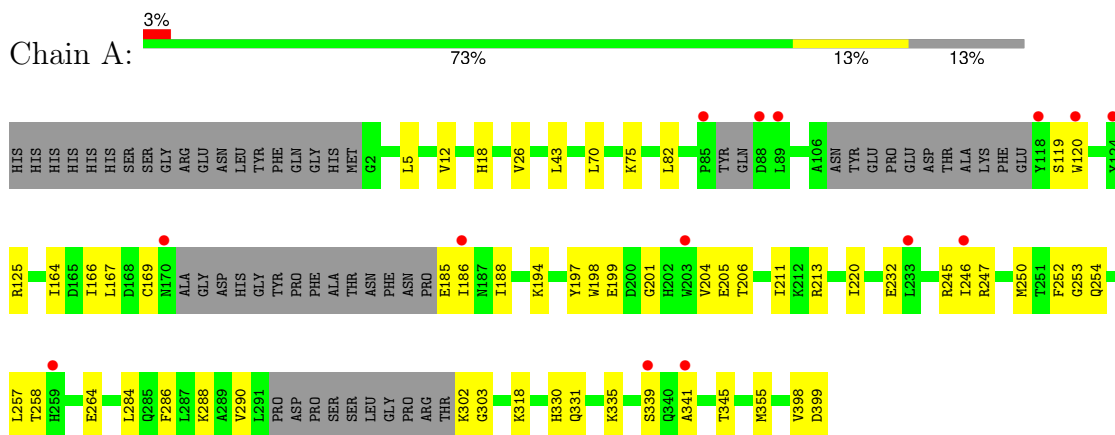
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	4	Total	O	0	0
			4	4		

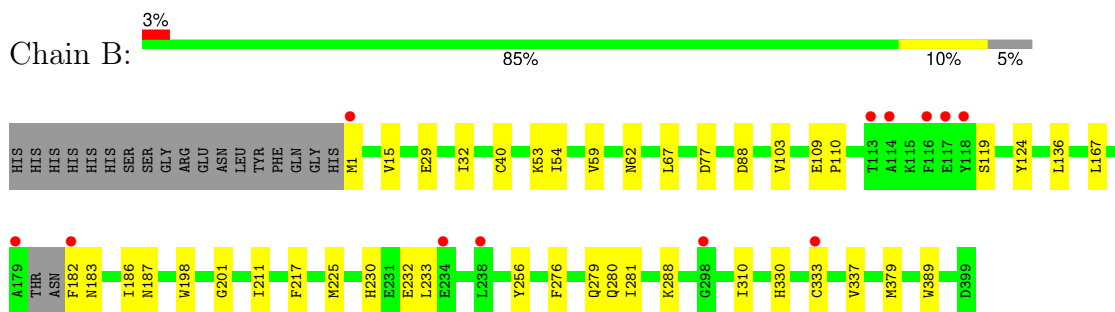
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

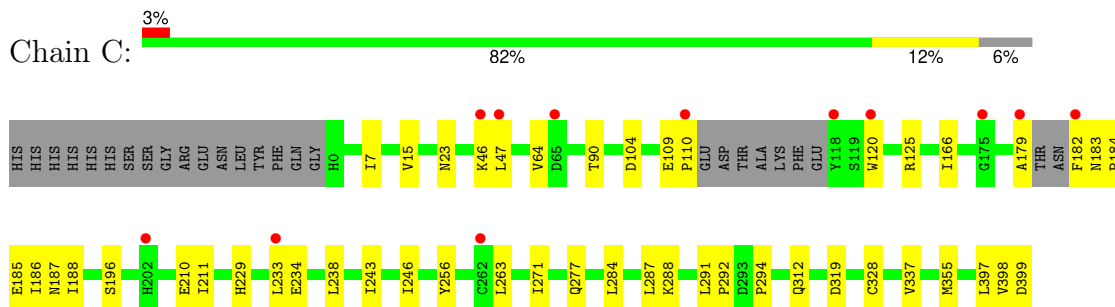
- Molecule 1: Saccharopine dehydrogenase



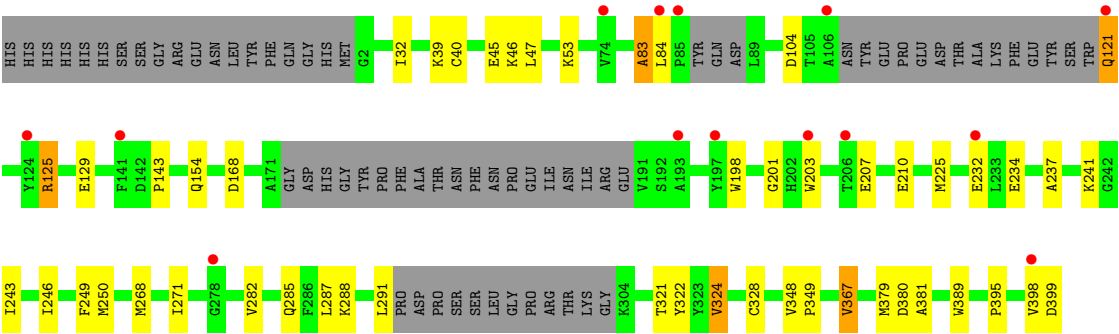
- Molecule 1: Saccharopine dehydrogenase



- Molecule 1: Saccharopine dehydrogenase



- Molecule 1: Saccharopine dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.93Å 65.24Å 156.52Å 94.91° 96.03° 90.04°	Depositor
Resolution (Å)	38.86 – 2.50 38.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.5 (38.86-2.50) 92.7 (38.86-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.205 , 0.251 0.209 , 0.255	Depositor DCC
R_{free} test set	1997 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21890	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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

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	0.16	0/2891	0.31	0/3906
1	B	0.16	0/3193	0.30	0/4325
1	C	0.17	0/3144	0.32	0/4258
1	D	0.23	0/2787	0.40	0/3766
All	All	0.18	0/12015	0.34	0/16255

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	125	ARG	Sidechain

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	2831	2389	2787	45	0
1	B	3117	2817	3040	30	0
1	C	3069	2639	2996	38	0
1	D	2730	2205	2695	38	0
2	B	6	8	8	0	0
2	C	6	8	8	0	0
3	A	7	0	0	0	0
3	B	28	0	0	0	0
3	C	26	0	0	0	0
3	D	4	0	0	0	0
All	All	11824	10066	11534	151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (151) 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:D:285:GLN:HA	1:D:288:LYS:HE2	1.26	1.10
1:B:232:GLU:N	1:B:232:GLU:OE1	2.08	0.86
1:A:185:GLU:N	1:A:185:GLU:OE1	2.15	0.79
1:A:254:GLN:OE1	1:A:258:THR:HG23	1.87	0.73
1:A:253:GLY:O	1:A:257:LEU:HD12	1.90	0.72
1:C:64:VAL:HG22	1:C:90:THR:HG23	1.75	0.68
1:A:12:VAL:HG12	1:A:82:LEU:HD13	1.75	0.68
1:D:282:VAL:CG1	1:D:285:GLN:HB2	2.24	0.67
1:C:263:LEU:HD13	1:C:287:LEU:HD21	1.78	0.66
1:A:164:ILE:HB	1:A:246:ILE:HD13	1.77	0.65
1:D:380:ASP:OD1	1:D:381:ALA:N	2.29	0.65
1:D:285:GLN:HA	1:D:288:LYS:CE	2.15	0.63
1:C:184:PRO:HD2	1:C:288:LYS:HE3	1.81	0.63
1:B:330:HIS:O	1:B:333:CYS:SG	2.52	0.62
1:D:243:ILE:HG12	1:D:246:ILE:HD11	1.80	0.62
1:A:286:PHE:O	1:A:290:VAL:HG23	2.00	0.62
1:C:312:GLN:OE1	1:C:397:LEU:HD13	2.01	0.61
1:D:83:ALA:C	1:D:84:LEU:HD22	2.25	0.61
1:B:119:SER:HA	1:B:124:TYR:CD2	2.35	0.61
1:A:185:GLU:N	1:A:188:ILE:HG13	2.16	0.60
1:C:184:PRO:HD2	1:C:288:LYS:CE	2.31	0.60
1:D:143:PRO:HB3	1:D:232:GLU:HG3	1.83	0.60
1:A:252:PHE:HB3	1:A:257:LEU:HD11	1.84	0.59
1:B:1:MET:HG2	1:B:77:ASP:CG	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ASN:ND2	1:C:355:MET:HE2	2.17	0.58
1:D:203:TRP:HZ2	1:D:234:GLU:HB2	1.68	0.58
1:D:207:GLU:HB2	1:D:210:GLU:OE1	2.04	0.57
1:C:182:PHE:N	1:C:294:PRO:HB3	2.20	0.57
1:A:247:ARG:NH2	1:A:398:VAL:HG13	2.20	0.57
1:C:319:ASP:C	1:C:319:ASP:OD1	2.48	0.57
1:C:398:VAL:O	1:C:399:ASP:HB2	2.05	0.56
1:C:184:PRO:O	1:C:188:ILE:HG22	2.05	0.56
1:A:254:GLN:OE1	1:A:254:GLN:O	2.24	0.56
1:A:18:HIS:HE1	1:A:43:LEU:HD11	1.71	0.55
1:D:322:TYR:CZ	1:D:324:VAL:HG22	2.41	0.55
1:D:268:MET:HE3	1:D:287:LEU:HB2	1.88	0.55
1:A:213:ARG:HH11	1:A:399:ASP:HA	1.71	0.55
1:A:199:GLU:HG3	1:A:245:ARG:HG2	1.89	0.54
1:C:211:ILE:HD12	1:C:211:ILE:N	2.23	0.54
1:A:185:GLU:HG2	1:A:186:ILE:H	1.73	0.53
1:B:109:GLU:HG2	1:B:110:PRO:HD2	1.91	0.53
1:C:179:ALA:O	1:C:291:LEU:HD13	2.08	0.53
1:C:196:SER:OG	1:C:229:HIS:ND1	2.32	0.53
1:A:284:LEU:O	1:A:288:LYS:HG3	2.09	0.53
1:A:188:ILE:HG21	1:A:264:GLU:OE1	2.09	0.53
1:D:398:VAL:HG12	1:D:398:VAL:O	2.09	0.52
1:B:167:LEU:HD11	1:B:310:ILE:HD11	1.91	0.52
1:C:182:PHE:O	1:C:184:PRO:HD3	2.10	0.52
1:B:379:MET:HE3	1:B:389:TRP:CE2	2.44	0.52
1:C:291:LEU:HB3	1:C:292:PRO:HD2	1.90	0.52
1:A:232:GLU:OE1	1:A:232:GLU:N	2.43	0.52
1:D:287:LEU:O	1:D:291:LEU:HG	2.10	0.52
1:C:284:LEU:O	1:C:284:LEU:HD23	2.11	0.51
1:A:250:MET:HE2	1:A:252:PHE:CZ	2.46	0.51
1:D:321:THR:HG23	1:D:395:PRO:HD2	1.92	0.51
1:A:398:VAL:O	1:A:399:ASP:HB3	2.11	0.51
1:D:282:VAL:HG13	1:D:285:GLN:HB2	1.91	0.51
1:C:319:ASP:OD1	1:C:319:ASP:O	2.29	0.51
1:D:348:VAL:HG12	1:D:349:PRO:HD3	1.93	0.50
1:B:167:LEU:HD22	1:B:225:MET:HE1	1.94	0.50
1:A:250:MET:HE2	1:A:252:PHE:CE2	2.47	0.49
1:C:398:VAL:O	1:C:399:ASP:CB	2.60	0.49
1:A:398:VAL:O	1:A:399:ASP:CB	2.61	0.49
1:A:119:SER:HG	1:A:120:TRP:CD1	2.29	0.49
1:C:185:GLU:HA	1:C:188:ILE:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ILE:HD12	1:B:211:ILE:N	2.27	0.49
1:D:348:VAL:N	1:D:349:PRO:HD2	2.28	0.49
1:B:182:PHE:O	1:B:288:LYS:NZ	2.46	0.49
1:C:187:ASN:HB3	1:C:256:TYR:OH	2.13	0.49
1:A:250:MET:CE	1:A:252:PHE:CZ	2.96	0.48
1:D:154:GLN:OE1	1:D:241:LYS:HG2	2.13	0.48
1:D:398:VAL:C	1:D:399:ASP:OD1	2.56	0.48
1:A:245:ARG:HD2	1:A:247:ARG:HG3	1.95	0.48
1:A:185:GLU:HG2	1:A:186:ILE:N	2.29	0.48
1:A:247:ARG:HH12	1:A:399:ASP:HB2	1.79	0.48
1:A:194:LYS:HG3	1:A:206:THR:O	2.14	0.48
1:C:182:PHE:CE1	1:C:186:ILE:HD12	2.48	0.48
1:D:168:ASP:OD2	1:D:250:MET:HE2	2.14	0.48
1:B:53:LYS:HD3	1:B:54:ILE:N	2.29	0.47
1:A:197:TYR:CZ	1:A:204:VAL:HG11	2.49	0.47
1:A:341:ALA:O	1:A:345:THR:HG23	2.14	0.47
1:A:398:VAL:HG22	1:A:399:ASP:N	2.29	0.47
1:B:119:SER:HA	1:B:124:TYR:HD2	1.77	0.47
1:D:168:ASP:OD2	1:D:250:MET:CE	2.63	0.47
1:B:103:VAL:HG13	1:B:136:LEU:HD23	1.96	0.47
1:B:276:PHE:HB3	1:B:281:ILE:HD12	1.97	0.47
1:C:210:GLU:HB3	1:C:211:ILE:HD12	1.98	0.46
1:C:277:GLN:O	1:C:277:GLN:CG	2.63	0.46
1:D:271:ILE:HA	1:D:282:VAL:CG2	2.45	0.46
1:B:279:GLN:HG2	1:B:280:GLN:N	2.30	0.46
1:A:185:GLU:HG2	1:A:186:ILE:HG22	1.98	0.46
1:D:237:ALA:HA	1:D:243:ILE:HG21	1.97	0.46
1:A:198:TRP:CZ2	1:A:201:GLY:HA2	2.50	0.46
1:D:83:ALA:O	1:D:84:LEU:HD22	2.15	0.46
1:D:46:LYS:HG2	1:D:47:LEU:HG	1.98	0.46
1:B:167:LEU:HD11	1:B:310:ILE:CD1	2.45	0.46
1:D:121:GLN:HE21	1:D:121:GLN:HB2	1.57	0.46
1:B:53:LYS:HD3	1:B:53:LYS:C	2.41	0.45
1:D:198:TRP:CZ2	1:D:201:GLY:HA2	2.51	0.45
1:A:5:LEU:HD21	1:A:70:LEU:HD12	1.98	0.45
1:D:321:THR:CG2	1:D:395:PRO:HD2	2.47	0.45
1:A:169:CYS:SG	1:A:220:ILE:HD13	2.57	0.45
1:B:230:HIS:HB3	1:B:233:LEU:HD13	1.98	0.45
1:B:1:MET:HA	1:B:77:ASP:OD2	2.17	0.45
1:B:32:ILE:HG13	1:B:40:CYS:HB3	1.97	0.45
1:A:194:LYS:HE3	1:A:205:GLU:OE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:VAL:HG22	1:B:337:VAL:HG21	1.98	0.44
1:A:211:ILE:HG23	1:A:213:ARG:NH2	2.32	0.44
1:A:185:GLU:N	1:A:188:ILE:CG1	2.81	0.44
1:B:62:ASN:OD1	1:B:88:ASP:OD2	2.36	0.43
1:C:120:TRP:HA	1:C:125:ARG:HD3	2.00	0.43
1:D:125:ARG:HG2	1:D:367:VAL:HG22	2.00	0.43
1:C:46:LYS:HG2	1:C:47:LEU:HD23	2.00	0.43
1:C:233:LEU:HD13	1:C:246:ILE:HG22	2.00	0.43
1:C:182:PHE:CD1	1:C:186:ILE:HD12	2.53	0.43
1:A:247:ARG:HH22	1:A:399:ASP:HB2	1.83	0.43
1:C:234:GLU:O	1:C:238:LEU:HG	2.19	0.43
1:D:32:ILE:HG13	1:D:40:CYS:HB3	2.01	0.42
1:B:29:GLU:HG2	1:B:53:LYS:HB3	2.01	0.42
1:A:302:LYS:CG	1:A:303:GLY:H	2.32	0.42
1:B:217:PHE:CZ	1:B:225:MET:HE3	2.53	0.42
1:A:166:ILE:O	1:A:167:LEU:HD12	2.20	0.42
1:D:380:ASP:OD1	1:D:380:ASP:C	2.61	0.42
1:C:15:VAL:HG22	1:C:337:VAL:HG21	2.02	0.42
1:C:183:ASN:OD1	1:C:185:GLU:HG2	2.19	0.42
1:B:59:VAL:HG21	1:B:67:LEU:HD23	2.02	0.42
1:D:53:LYS:O	1:D:53:LYS:HG3	2.19	0.42
1:D:285:GLN:HG3	1:D:288:LYS:NZ	2.35	0.42
1:A:211:ILE:N	1:A:211:ILE:HD12	2.35	0.42
1:B:198:TRP:CZ2	1:B:201:GLY:HA2	2.55	0.42
1:C:7:ILE:HD12	1:C:7:ILE:N	2.35	0.42
1:A:331:GLN:HG2	1:A:335:LYS:CE	2.50	0.41
1:B:330:HIS:HA	1:B:333:CYS:SG	2.59	0.41
1:D:282:VAL:HG13	1:D:285:GLN:H	1.85	0.41
1:C:23:ASN:HD21	1:C:355:MET:HE2	1.83	0.41
1:A:26:VAL:HG21	1:A:355:MET:SD	2.61	0.41
1:C:183:ASN:CG	1:C:185:GLU:HG2	2.44	0.41
1:A:330:HIS:CE1	1:A:341:ALA:HB3	2.56	0.41
1:C:104:ASP:OD1	1:C:104:ASP:C	2.63	0.41
1:D:104:ASP:OD1	1:D:104:ASP:C	2.63	0.41
1:D:225:MET:HE3	1:D:249:PHE:CG	2.55	0.41
1:C:243:ILE:HG12	1:C:246:ILE:HD11	2.03	0.41
1:B:187:ASN:HB3	1:B:256:TYR:OH	2.21	0.41
1:C:166:ILE:HD12	1:C:233:LEU:HD21	2.03	0.41
1:D:398:VAL:O	1:D:398:VAL:CG1	2.68	0.41
1:C:109:GLU:OE2	1:C:110:PRO:HD2	2.21	0.41
1:D:379:MET:HE3	1:D:389:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASN:ND2	1:B:62:ASN:O	2.53	0.40
1:C:271:ILE:HD12	1:C:271:ILE:C	2.46	0.40
1:A:120:TRP:HA	1:A:125:ARG:HD2	2.03	0.40
1:B:183:ASN:HB3	1:B:186:ILE:HD11	2.04	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	351/417 (84%)	343 (98%)	8 (2%)	0	100	100
1	B	393/417 (94%)	382 (97%)	11 (3%)	0	100	100
1	C	385/417 (92%)	378 (98%)	7 (2%)	0	100	100
1	D	340/417 (82%)	327 (96%)	12 (4%)	1 (0%)	36	55
All	All	1469/1668 (88%)	1430 (97%)	38 (3%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	83	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/354 (86%)	303 (99%)	3 (1%)	68	86
1	B	336/354 (95%)	336 (100%)	0	100	100
1	C	331/354 (94%)	330 (100%)	1 (0%)	86	94
1	D	295/354 (83%)	288 (98%)	7 (2%)	43	70
All	All	1268/1416 (90%)	1257 (99%)	11 (1%)	70	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	318	LYS
1	A	339	SER
1	C	328	CYS
1	D	39	LYS
1	D	45	GLU
1	D	121	GLN
1	D	129	GLU
1	D	324	VAL
1	D	328	CYS
1	D	367	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	ASN
1	B	202	HIS
1	C	62	ASN
1	D	62	ASN
1	D	121	GLN
1	D	162	ASN
1	D	259	HIS
1	D	279	GLN
1	D	312	GLN
1	D	330	HIS

5.3.3 RNA ⓘ

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](#)

2 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	GOL	B	401	-	5,5,5	0.32	0	5,5,5	0.42	0
2	GOL	C	401	-	5,5,5	0.33	0	5,5,5	0.36	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
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	C	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	GOL	O1-C1-C2-C3
2	B	401	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	361/417 (86%)	0.56	14 (3%) 43 38	42, 64, 89, 97	0
1	B	397/417 (95%)	0.16	12 (3%) 52 48	29, 49, 79, 108	0
1	C	391/417 (93%)	0.19	12 (3%) 51 47	30, 50, 77, 97	0
1	D	350/417 (83%)	0.52	14 (4%) 42 38	30, 61, 80, 91	0
All	All	1499/1668 (89%)	0.35	52 (3%) 47 42	29, 57, 83, 108	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	118	TYR	5.8
1	C	179	ALA	4.9
1	A	118	TYR	4.7
1	C	182	PHE	4.4
1	B	116	PHE	4.0
1	D	193	ALA	3.5
1	B	118	TYR	3.5
1	B	298	GLY	3.5
1	A	120	TRP	3.4
1	B	333	CYS	3.3
1	B	1	MET	3.1
1	C	110	PRO	3.1
1	B	182	PHE	3.0
1	A	186	ILE	3.0
1	A	88	ASP	2.8
1	D	85	PRO	2.7
1	D	124	TYR	2.7
1	D	141	PHE	2.7
1	D	232	GLU	2.7
1	B	114	ALA	2.7
1	A	203	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	85	PRO	2.5
1	D	74	VAL	2.5
1	A	170	ASN	2.5
1	D	398	VAL	2.5
1	A	89	LEU	2.5
1	C	202	HIS	2.5
1	C	262	CYS	2.4
1	D	278	GLY	2.4
1	C	233	LEU	2.3
1	B	179	ALA	2.3
1	A	339	SER	2.3
1	A	259	HIS	2.3
1	B	117	GLU	2.3
1	B	234	GLU	2.2
1	C	47	LEU	2.2
1	D	206	THR	2.2
1	A	124	TYR	2.2
1	D	106	ALA	2.1
1	B	238	LEU	2.1
1	A	246	ILE	2.1
1	A	341	ALA	2.1
1	C	120	TRP	2.1
1	C	175	GLY	2.1
1	D	197	TYR	2.1
1	D	121	GLN	2.1
1	A	233	LEU	2.1
1	B	113	THR	2.0
1	D	203	TRP	2.0
1	C	46	LYS	2.0
1	D	84	LEU	2.0
1	C	65	ASP	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
2	GOL	C	401	6/6	0.84	0.15	53,64,73,74	0
2	GOL	B	401	6/6	0.85	0.17	52,62,73,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.