



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:57 PM EDT

PDB ID : 6DA6 / pdb_00006da6
Title : Crystal structure of the TtnD decarboxylase from the tautomycetin biosynthesis pathway of *Streptomyces griseochromogenes*, apo form at 2.6 Å resolution (P212121)
Authors : Han, L.; Rudolf, J.D.; Chang, C.-Y.; Miller, M.D.; Soman, J.; Phillips Jr., G.N.; Shen, B.; Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on : 2018-05-01
Resolution : 2.59 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	:	9.0.010 (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

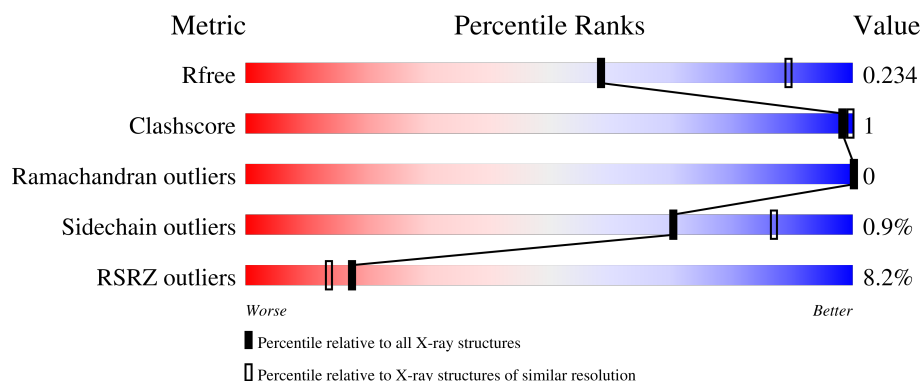
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	501	11% 91% 7%
1	B	501	89% 7%
1	C	501	11% 90% 8%
1	D	501	18% 89% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14555 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 UbiD-like decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3557	2259	624	656	18			
1	B	464	Total	C	N	O	S	0	0	0
			3557	2259	624	656	18			
1	C	463	Total	C	N	O	S	0	0	0
			3552	2257	623	654	18			
1	D	461	Total	C	N	O	S	0	0	0
			3539	2249	621	652	17			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP C6ZCR8
A	-14	GLY	-	expression tag	UNP C6ZCR8
A	-13	SER	-	expression tag	UNP C6ZCR8
A	-12	SER	-	expression tag	UNP C6ZCR8
A	-11	HIS	-	expression tag	UNP C6ZCR8
A	-10	HIS	-	expression tag	UNP C6ZCR8
A	-9	HIS	-	expression tag	UNP C6ZCR8
A	-8	HIS	-	expression tag	UNP C6ZCR8
A	-7	HIS	-	expression tag	UNP C6ZCR8
A	-6	HIS	-	expression tag	UNP C6ZCR8
A	-5	SER	-	expression tag	UNP C6ZCR8
A	-4	GLN	-	expression tag	UNP C6ZCR8
A	-3	ASP	-	expression tag	UNP C6ZCR8
A	-2	PRO	-	expression tag	UNP C6ZCR8
A	-1	ASN	-	expression tag	UNP C6ZCR8
A	0	SER	-	expression tag	UNP C6ZCR8
B	-15	MET	-	initiating methionine	UNP C6ZCR8
B	-14	GLY	-	expression tag	UNP C6ZCR8
B	-13	SER	-	expression tag	UNP C6ZCR8
B	-12	SER	-	expression tag	UNP C6ZCR8
B	-11	HIS	-	expression tag	UNP C6ZCR8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP C6ZCR8
B	-9	HIS	-	expression tag	UNP C6ZCR8
B	-8	HIS	-	expression tag	UNP C6ZCR8
B	-7	HIS	-	expression tag	UNP C6ZCR8
B	-6	HIS	-	expression tag	UNP C6ZCR8
B	-5	SER	-	expression tag	UNP C6ZCR8
B	-4	GLN	-	expression tag	UNP C6ZCR8
B	-3	ASP	-	expression tag	UNP C6ZCR8
B	-2	PRO	-	expression tag	UNP C6ZCR8
B	-1	ASN	-	expression tag	UNP C6ZCR8
B	0	SER	-	expression tag	UNP C6ZCR8
C	-15	MET	-	initiating methionine	UNP C6ZCR8
C	-14	GLY	-	expression tag	UNP C6ZCR8
C	-13	SER	-	expression tag	UNP C6ZCR8
C	-12	SER	-	expression tag	UNP C6ZCR8
C	-11	HIS	-	expression tag	UNP C6ZCR8
C	-10	HIS	-	expression tag	UNP C6ZCR8
C	-9	HIS	-	expression tag	UNP C6ZCR8
C	-8	HIS	-	expression tag	UNP C6ZCR8
C	-7	HIS	-	expression tag	UNP C6ZCR8
C	-6	HIS	-	expression tag	UNP C6ZCR8
C	-5	SER	-	expression tag	UNP C6ZCR8
C	-4	GLN	-	expression tag	UNP C6ZCR8
C	-3	ASP	-	expression tag	UNP C6ZCR8
C	-2	PRO	-	expression tag	UNP C6ZCR8
C	-1	ASN	-	expression tag	UNP C6ZCR8
C	0	SER	-	expression tag	UNP C6ZCR8
D	-15	MET	-	initiating methionine	UNP C6ZCR8
D	-14	GLY	-	expression tag	UNP C6ZCR8
D	-13	SER	-	expression tag	UNP C6ZCR8
D	-12	SER	-	expression tag	UNP C6ZCR8
D	-11	HIS	-	expression tag	UNP C6ZCR8
D	-10	HIS	-	expression tag	UNP C6ZCR8
D	-9	HIS	-	expression tag	UNP C6ZCR8
D	-8	HIS	-	expression tag	UNP C6ZCR8
D	-7	HIS	-	expression tag	UNP C6ZCR8
D	-6	HIS	-	expression tag	UNP C6ZCR8
D	-5	SER	-	expression tag	UNP C6ZCR8
D	-4	GLN	-	expression tag	UNP C6ZCR8
D	-3	ASP	-	expression tag	UNP C6ZCR8
D	-2	PRO	-	expression tag	UNP C6ZCR8
D	-1	ASN	-	expression tag	UNP C6ZCR8

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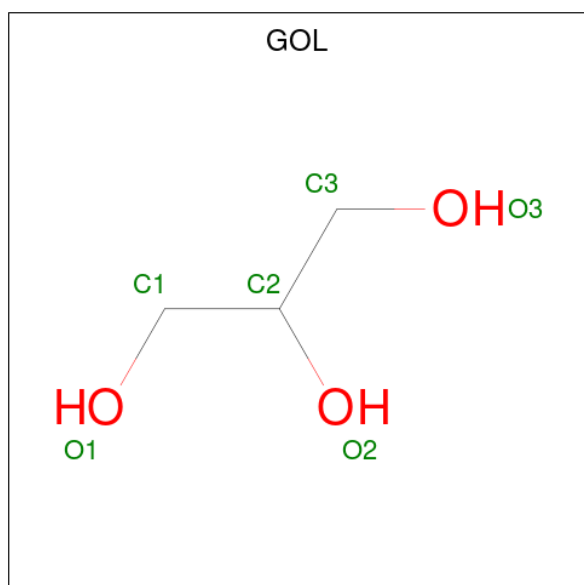
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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP C6ZCR8

- 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	D	1	Total Mg 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 4 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O 9 9	0	0
4	D	1	Total O 9 9	0	0

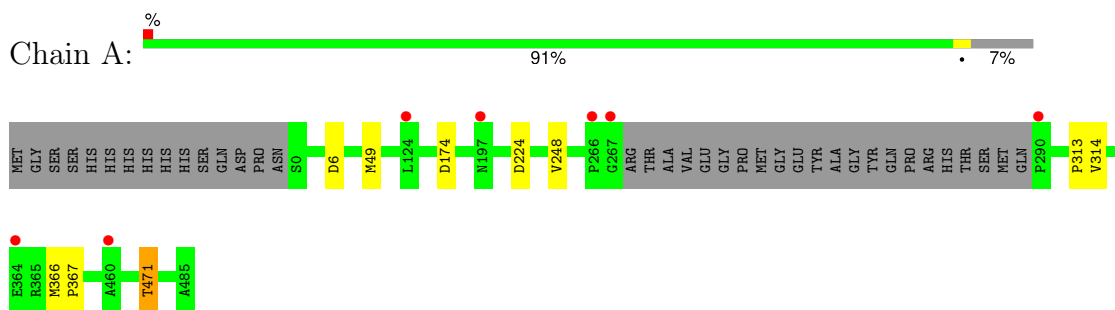
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	74	Total O 74 74	0	0
5	B	70	Total O 70 70	0	0
5	C	44	Total O 44 44	0	0
5	D	45	Total O 45 45	0	0

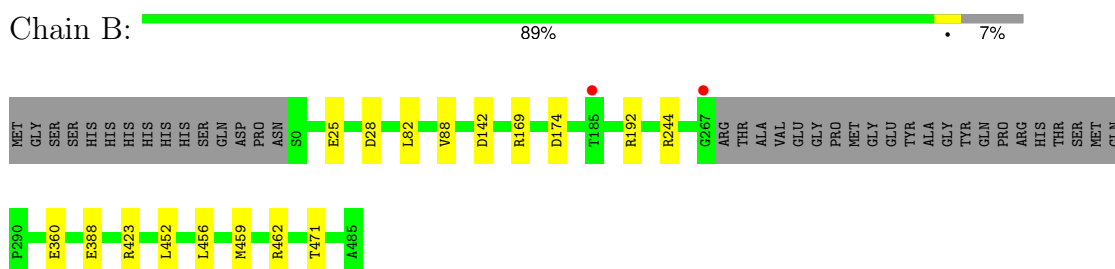
3 Residue-property plots

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.

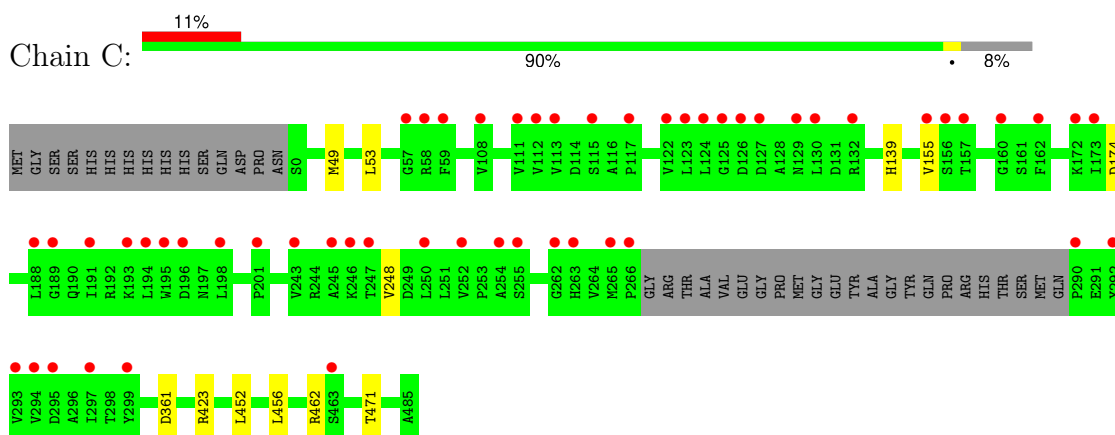
- Molecule 1: UbiD-like decarboxylase



- Molecule 1: UbiD-like decarboxylase



- Molecule 1: UbiD-like decarboxylase



- Molecule 1: UbiD-like decarboxylase

GLY	ARG	T154	GLY	MET
THR	THR	T155	GLY	GLY
ALA	VAL	T156	SER	SER
VAL	VAL	T157	SER	SER
GLU	GLU	T158	HIS	HIS
GLY	GLY	T159	HIS	HIS
PRO	PRO	T160	HIS	HIS
PRO	PRO	T161	HIS	HIS
MET	MET	T162	HIS	HIS
GLY	GLY	T163	SER	SER
GLU	GLU	T173	GLN	GLN
TYR	TYR	T174	ASP	ASP
GLY	GLY	T175	PRO	PRO
TYR	TYR	T182	ASN	ASN
GLN	GLN	T183	SER	SER
PRO	PRO	T188	MET	MET
ARG	ARG	T191	Y2	Y2
HIS	HIS	T192	Y23	Y23
THR	THR	T193	Y51	Y51
SER	SER	T194	Y53	Y53
MET	MET	T195	Y54	Y54
GLN	GLN	T196	Y55	Y55
Y280	Y281	T197	Y56	Y56
Y292	Y293	T198	Y57	Y57
Y293	Y294	T199	Y58	Y58
Y295	Y296	T200	Y59	Y59
Y296	Y297	T201	Y60	Y60
Y298	Y299	T202	Y61	Y61
Y299	Y300	T203	Y62	Y62
Y300	Y301	T204	Y111	Y111
Y302	Y303	T242	Y112	Y112
Y304	Y304	T243	Y113	Y113
Y367	Y367	T244	Y116	Y116
Y423	Y423	T245	Y117	Y117
Y452	Y452	T246	Y118	Y118
Y456	Y456	T247	Y119	Y119
Y459	Y459	T248	Y120	Y120
Y460	Y461	T249	Y121	Y121
Y462	Y462	T250	Y122	Y122
Y471	Y471	T251	Y123	Y123
Y485	Y485	T252	Y124	Y124
		T253	Y125	Y125
		T254	Y128	Y128
		T255	Y129	Y129
		T256	Y130	Y130
		T257	Y131	Y131
		T258	Y132	Y132
		T259	Y133	Y133
		T260	Y134	Y134
		T261	Y135	Y135
		T262	Y152	Y152
		T263	Y153	Y153
		T264	Y154	Y154
		T265	Y155	Y155

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.22Å 137.12Å 284.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.13 – 2.59 26.13 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (26.13-2.59) 99.6 (26.13-2.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.60Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.195 , 0.227 0.202 , 0.234	Depositor DCC
R_{free} test set	1998 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14555	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: UNL, MG, 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	0.88	2/3644 (0.1%)	1.05	7/4977 (0.1%)
1	B	0.90	1/3644 (0.0%)	1.07	2/4977 (0.0%)
1	C	0.81	1/3639 (0.0%)	1.04	3/4971 (0.1%)
1	D	0.80	0/3626	1.04	1/4954 (0.0%)
All	All	0.85	4/14553 (0.0%)	1.05	13/19879 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	MET	SD-CE	-7.55	1.60	1.79
1	C	49	MET	SD-CE	-5.89	1.64	1.79
1	B	28	ASP	CA-C	5.59	1.59	1.52
1	A	366	MET	SD-CE	-5.06	1.67	1.79

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	VAL	N-CA-C	7.18	124.28	109.34
1	C	248	VAL	N-CA-C	5.68	121.15	109.34
1	A	6	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	174	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	224	ASP	N-CA-C	5.28	117.44	111.11
1	A	174	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	367	PRO	N-CA-C	5.21	120.68	113.65
1	A	248	VAL	CA-C-O	-5.12	114.37	120.78
1	A	248	VAL	CB-CA-C	-5.12	102.89	111.29
1	B	142	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	174	ASP	CA-CB-CG	5.11	117.71	112.60
1	C	361	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	367	PRO	N-CA-C	5.03	120.44	113.65

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	3557	0	3555	2	0
1	B	3557	0	3555	5	0
1	C	3552	0	3549	4	0
1	D	3539	0	3535	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	36	0	48	0	0
3	B	30	0	40	0	0
3	C	24	0	32	0	0
3	D	6	0	8	0	0
4	C	9	0	0	1	0
4	D	9	0	0	1	0
5	A	74	0	0	0	0
5	B	70	0	0	0	0
5	C	44	0	0	0	0
5	D	45	0	0	0	0
All	All	14555	0	14322	18	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 1.

All (18) 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)
4:D:502:UNL:O7	4:D:502:UNL:O1	1.56	1.24
4:C:505:UNL:O1	4:C:505:UNL:O7	1.57	1.21
1:D:116:ALA:HB2	1:D:243:VAL:HG21	1.90	0.53
1:B:360:GLU:OE2	1:B:459:MET:HE3	2.12	0.49
1:B:456:LEU:HD13	1:B:462:ARG:HD3	1.94	0.49
1:D:59:PHE:CE2	1:D:133:PHE:CE1	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:THR:HG22	1:D:471:THR:O	2.14	0.47
1:B:82:LEU:HD21	1:B:88:VAL:HG13	1.96	0.47
1:C:456:LEU:HD13	1:C:462:ARG:HD3	1.97	0.47
1:A:471:THR:HG21	1:C:139:HIS:HB3	1.98	0.45
1:D:423:ARG:HG3	1:D:452:LEU:CD1	2.47	0.45
1:D:456:LEU:HD13	1:D:462:ARG:HD3	1.98	0.45
1:B:423:ARG:HG3	1:B:452:LEU:CD1	2.48	0.44
1:C:423:ARG:HG3	1:C:452:LEU:CD1	2.49	0.42
1:D:423:ARG:HG3	1:D:452:LEU:HD13	2.01	0.42
1:B:423:ARG:HG3	1:B:452:LEU:HD13	2.01	0.41
1:A:313:PRO:HA	1:A:314:VAL:HA	1.87	0.41
1:C:423:ARG:HG3	1:C:452:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

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	460/501 (92%)	448 (97%)	12 (3%)	0	100	100
1	B	460/501 (92%)	450 (98%)	10 (2%)	0	100	100
1	C	459/501 (92%)	443 (96%)	16 (4%)	0	100	100
1	D	457/501 (91%)	445 (97%)	12 (3%)	0	100	100
All	All	1836/2004 (92%)	1786 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	374/405 (92%)	373 (100%)	1 (0%)	86	94
1	B	374/405 (92%)	368 (98%)	6 (2%)	55	79
1	C	373/405 (92%)	370 (99%)	3 (1%)	73	88
1	D	372/405 (92%)	368 (99%)	4 (1%)	65	84
All	All	1493/1620 (92%)	1479 (99%)	14 (1%)	70	87

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	471	THR
1	B	25	GLU
1	B	169	ARG
1	B	192	ARG
1	B	244	ARG
1	B	388	GLU
1	B	471	THR
1	C	53	LEU
1	C	155	VAL
1	C	471	THR
1	D	62	ILE
1	D	152	THR
1	D	155	VAL
1	D	265	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	HIS
1	B	200	GLN
1	C	43	ASN
1	C	51	ASN
1	C	121	ASN
1	D	164	ASN

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 21 ligands modelled in this entry, 3 are monoatomic and 2 are unknown - leaving 16 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	$\# Z > 2$
3	GOL	C	502	-	5,5,5	0.11	0	5,5,5	0.32	0
3	GOL	B	503	-	5,5,5	0.28	0	5,5,5	0.25	0
3	GOL	C	501	-	5,5,5	0.22	0	5,5,5	0.76	0
3	GOL	B	504	-	5,5,5	0.18	0	5,5,5	0.36	0
3	GOL	D	501	-	5,5,5	0.25	0	5,5,5	0.32	0
3	GOL	A	502	-	5,5,5	0.28	0	5,5,5	0.37	0
3	GOL	C	504	-	5,5,5	0.33	0	5,5,5	0.47	0
3	GOL	A	505	-	5,5,5	0.15	0	5,5,5	0.23	0
3	GOL	C	503	-	5,5,5	0.16	0	5,5,5	0.38	0
3	GOL	A	503	-	5,5,5	0.06	0	5,5,5	0.29	0
3	GOL	B	505	-	5,5,5	0.08	0	5,5,5	0.18	0
3	GOL	A	506	-	5,5,5	0.15	0	5,5,5	0.43	0
3	GOL	A	507	-	5,5,5	0.16	0	5,5,5	0.13	0
3	GOL	B	502	-	5,5,5	0.08	0	5,5,5	0.52	0
3	GOL	A	504	-	5,5,5	0.55	0	5,5,5	0.79	0
3	GOL	B	501	-	5,5,5	0.10	0	5,5,5	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	502	-	-	0/4/4/4	-
3	GOL	B	503	-	-	1/4/4/4	-
3	GOL	C	501	-	-	0/4/4/4	-
3	GOL	B	504	-	-	0/4/4/4	-
3	GOL	D	501	-	-	0/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	C	504	-	-	0/4/4/4	-
3	GOL	A	505	-	-	2/4/4/4	-
3	GOL	C	503	-	-	1/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	B	505	-	-	0/4/4/4	-
3	GOL	A	506	-	-	2/4/4/4	-
3	GOL	A	507	-	-	2/4/4/4	-
3	GOL	B	502	-	-	0/4/4/4	-
3	GOL	A	504	-	-	2/4/4/4	-
3	GOL	B	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	GOL	O1-C1-C2-C3
3	A	505	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-O2
3	A	502	GOL	C1-C2-C3-O3
3	A	506	GOL	C1-C2-C3-O3
3	A	507	GOL	O1-C1-C2-C3
3	B	501	GOL	C1-C2-C3-O3
3	A	505	GOL	O2-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3
3	A	504	GOL	O2-C2-C3-O3
3	A	507	GOL	O1-C1-C2-O2
3	A	506	GOL	O2-C2-C3-O3
3	B	501	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	C	503	GOL	C1-C2-C3-O3
3	B	503	GOL	O2-C2-C3-O3
3	A	504	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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	464/501 (92%)	-0.18	7 (1%) 72 68	29, 47, 94, 118	0
1	B	464/501 (92%)	-0.37	2 (0%) 88 86	29, 47, 85, 124	0
1	C	463/501 (92%)	0.49	54 (11%) 9 7	31, 71, 175, 228	0
1	D	461/501 (92%)	0.70	89 (19%) 3 2	28, 75, 208, 254	0
All	All	1852/2004 (92%)	0.16	152 (8%) 17 14	28, 55, 176, 254	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	124	LEU	4.8
1	D	266	PRO	4.8
1	D	122	VAL	4.7
1	C	198	LEU	4.6
1	D	297	ILE	4.3
1	D	124	LEU	4.2
1	A	460	ALA	4.1
1	C	246	LYS	3.9
1	D	155	VAL	3.9
1	D	59	PHE	3.9
1	C	297	ILE	3.8
1	D	194	LEU	3.8
1	D	118	CYS	3.8
1	D	195	TRP	3.8
1	D	123	LEU	3.8
1	D	55	GLY	3.7
1	C	194	LEU	3.7
1	D	201	PRO	3.7
1	C	292	TYR	3.7
1	C	112	VAL	3.6
1	D	133	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	199	GLY	3.6
1	D	200	GLN	3.6
1	C	265	MET	3.5
1	D	112	VAL	3.5
1	C	125	GLY	3.5
1	D	135	ALA	3.5
1	C	247	THR	3.4
1	D	113	VAL	3.4
1	D	247	THR	3.4
1	D	198	LEU	3.4
1	C	290	PRO	3.4
1	D	117	PRO	3.4
1	D	125	GLY	3.4
1	D	111	VAL	3.3
1	D	293	VAL	3.3
1	C	57	GLY	3.3
1	C	123	LEU	3.3
1	D	132	ARG	3.3
1	D	290	PRO	3.3
1	D	191	ILE	3.3
1	D	203	PRO	3.3
1	D	264	VAL	3.2
1	D	292	TYR	3.2
1	D	54	THR	3.2
1	A	266	PRO	3.2
1	D	129	ASN	3.2
1	D	60	CYS	3.2
1	C	463	SER	3.1
1	C	188	LEU	3.1
1	C	122	VAL	3.1
1	D	265	MET	3.1
1	D	248	VAL	3.1
1	D	119	GLN	3.1
1	D	56	THR	3.1
1	D	260	ILE	3.1
1	D	298	THR	3.1
1	D	459	MET	3.1
1	D	163	THR	3.0
1	D	134	PRO	3.0
1	D	202	MET	3.0
1	D	261	GLU	3.0
1	C	113	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	51	ASN	3.0
1	D	158	PRO	2.9
1	C	294	VAL	2.9
1	C	266	PRO	2.9
1	C	250	LEU	2.9
1	D	121	ASN	2.9
1	D	295	ASP	2.8
1	D	204	PHE	2.8
1	D	243	VAL	2.8
1	C	59	PHE	2.8
1	A	197	ASN	2.8
1	A	267	GLY	2.7
1	D	258	ILE	2.7
1	D	162	PHE	2.7
1	D	251	LEU	2.7
1	D	130	LEU	2.7
1	D	188	LEU	2.7
1	D	299	TYR	2.7
1	D	256	ALA	2.7
1	D	294	VAL	2.7
1	D	128	ALA	2.7
1	B	267	GLY	2.6
1	D	460	ALA	2.6
1	C	299	TYR	2.6
1	D	153	ILE	2.6
1	D	116	ALA	2.6
1	D	262	GLY	2.5
1	C	132	ARG	2.5
1	D	120	ASP	2.5
1	D	53	LEU	2.5
1	D	175	GLY	2.5
1	C	193	LYS	2.5
1	D	160	GLY	2.5
1	C	127	ASP	2.5
1	C	173	ILE	2.5
1	D	173	ILE	2.5
1	D	197	ASN	2.5
1	C	254	ALA	2.5
1	C	111	VAL	2.4
1	C	243	VAL	2.4
1	D	301	ASP	2.4
1	D	245	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	196	ASP	2.4
1	C	263	HIS	2.4
1	D	192	ARG	2.4
1	C	115	SER	2.4
1	C	155	VAL	2.4
1	D	252	VAL	2.4
1	C	201	PRO	2.3
1	C	189	GLY	2.3
1	C	295	ASP	2.3
1	A	290	PRO	2.3
1	C	108	VAL	2.3
1	C	245	ALA	2.3
1	D	196	ASP	2.3
1	D	254	ALA	2.3
1	D	303	PRO	2.3
1	A	364	GLU	2.3
1	C	293	VAL	2.3
1	C	157	THR	2.2
1	A	124	LEU	2.2
1	D	183	ILE	2.2
1	C	126	ASP	2.2
1	D	193	LYS	2.2
1	D	242	LEU	2.2
1	D	131	ASP	2.2
1	C	130	LEU	2.2
1	C	160	GLY	2.2
1	C	262	GLY	2.2
1	D	156	SER	2.2
1	C	58	ARG	2.2
1	D	263	HIS	2.2
1	C	191	ILE	2.2
1	D	57	GLY	2.1
1	C	255	SER	2.1
1	D	302	ASP	2.1
1	C	172	LYS	2.1
1	D	246	LYS	2.1
1	D	182	PHE	2.1
1	C	156	SER	2.1
1	C	129	ASN	2.1
1	D	250	LEU	2.1
1	C	162	PHE	2.1
1	B	185	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	117	PRO	2.1
1	C	252	VAL	2.0
1	C	195	TRP	2.0
1	D	23	ILE	2.0
1	D	304	ILE	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
3	GOL	C	502	6/6	0.72	0.15	73,76,83,86	0
3	GOL	C	504	6/6	0.73	0.15	76,81,83,85	0
3	GOL	A	506	6/6	0.76	0.14	72,75,77,78	0
3	GOL	A	504	6/6	0.78	0.19	45,59,62,67	0
4	UNL	C	505	9/-	0.80	0.17	79,84,89,90	0
3	GOL	A	502	6/6	0.81	0.14	59,67,70,70	0
2	MG	D	503	1/1	0.81	0.24	73,73,73,73	0
4	UNL	D	502	9/-	0.82	0.15	80,82,86,87	0
3	GOL	B	504	6/6	0.84	0.18	62,75,79,79	0
3	GOL	A	505	6/6	0.85	0.16	64,66,70,73	0
3	GOL	D	501	6/6	0.85	0.17	67,78,79,84	0
3	GOL	B	503	6/6	0.87	0.12	66,69,70,71	0
3	GOL	A	503	6/6	0.89	0.13	58,66,71,72	0
3	GOL	B	505	6/6	0.91	0.13	66,71,73,75	0
3	GOL	C	501	6/6	0.92	0.12	55,61,68,72	0
3	GOL	B	501	6/6	0.92	0.08	52,53,56,59	0
3	GOL	C	503	6/6	0.93	0.08	56,57,59,63	0
2	MG	A	501	1/1	0.94	0.06	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	502	6/6	0.94	0.09	54,54,55,57	0
3	GOL	A	507	6/6	0.95	0.08	40,49,53,56	0
2	MG	B	506	1/1	0.97	0.04	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.