Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 01:42 PM EDT

PDB ID	:	6DA6
Title	:	Crystal structure of the TtnD decarboxylase from the tautomycetin biosynthesis pathway of Streptomyces griseochromogenes, apo form at 2.6 A 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 (i) 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 (i)) were used in the production of this report:

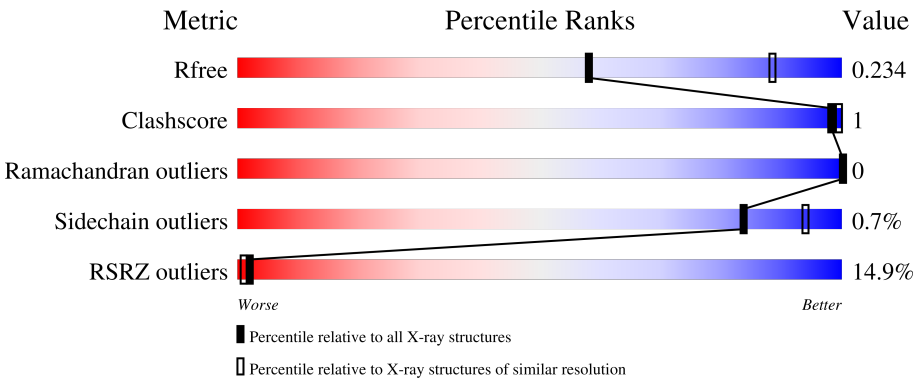
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	5% 92% 7%
1	B	501	6% 90% • 7%
1	C	501	17% 91% • 8%
1	D	501	27% 90% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	D	503	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	464	3557	2259	624	656	18	0	0	0
1	B	464	3557	2259	624	656	18	0	0	0
1	C	463	3552	2257	623	654	18	0	0	0
1	D	461	3539	2249	621	652	17	0	0	0

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

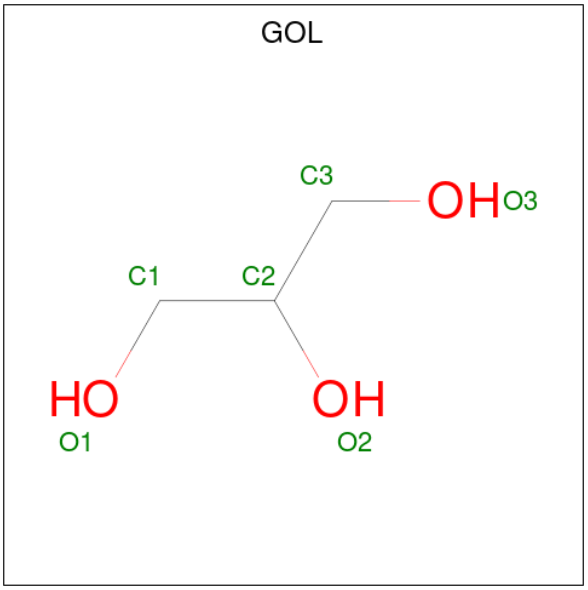
Continued from previous page...

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

- Molecule 2 is MAGNESIUM ION (three-letter code: 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

- Molecule 5 is water.

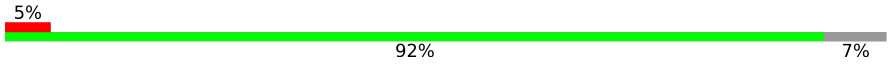
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	74	74	74	0	0
5	B	70	70	70	0	0
5	C	44	44	44	0	0
5	D	45	45	45	0	0

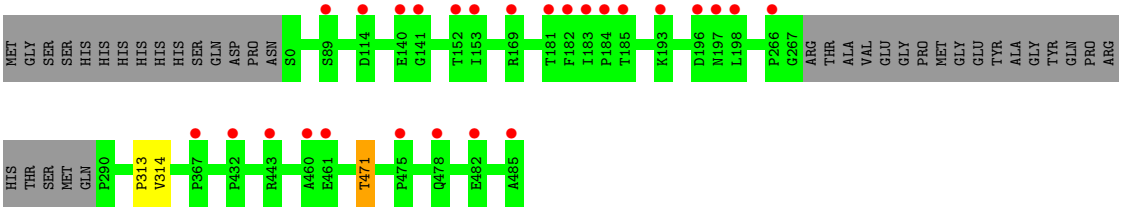
3 Residue-property plots (i)

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: UbiD-like decarboxylase

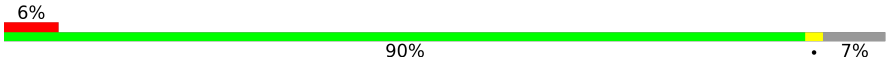
Chain A:

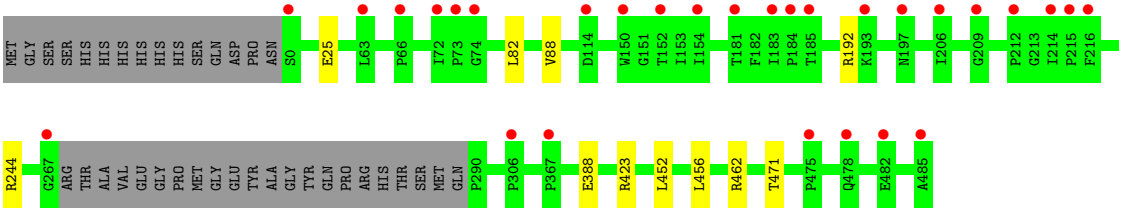




• Molecule 1: UbiD-like decarboxylase

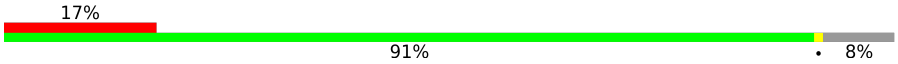
Chain B:

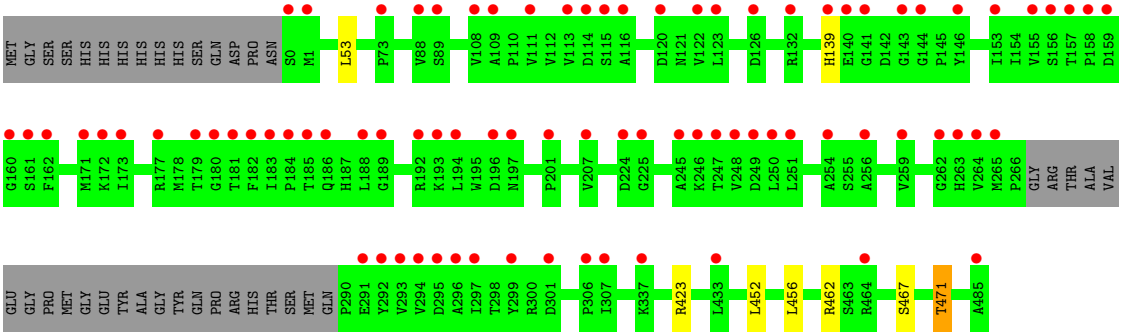




• Molecule 1: UbiD-like decarboxylase

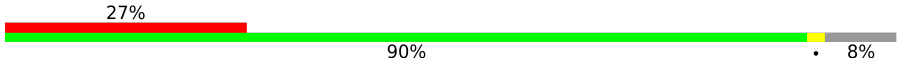
Chain C:

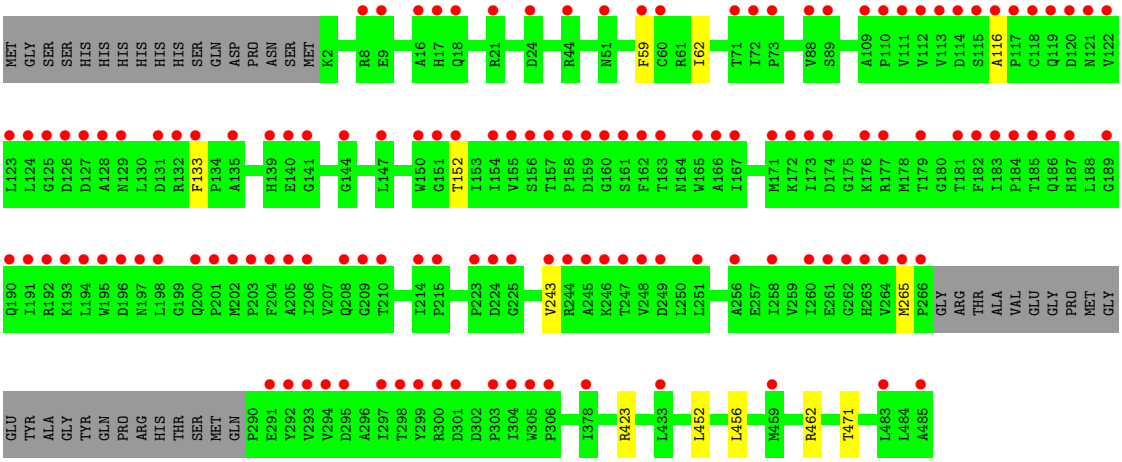




• Molecule 1: UbiD-like decarboxylase

Chain D:


27%
90%
8%


MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER GLN ASP PRO ASN SER MET K2 R8 E9 A16 H17 Q18 R21 D24 R44 N51 F59 C60 R61 I62 T71 I72 P73 V88 S89 A109 P110 V111 V112 V113 D114 S115 A116 P117 C118 Q119 D120 N121 V122
L123 L124 G125 D126 D127 A128 N129 L130 D131 R132 F133 P134 A135 H139 E140 G141 G144 L147 W150 G151 T152 I153 I154 V155 S156 T157 P158 D159 G160 S161 F162 T163 N164 W165 A166 I167 M171 K172 I173 D174 G175 K176 R177 M178 T179 G180 T181 F182 I183 P184 T185 Q186 H187 L188 G189
Q190 I191 R192 K193 L194 W195 D196 N197 L198 G199 Q200 P201 M202 P203 F204 A205 I206 V207 Q208 G209 T210 I214 P215 P223 D224 G225 V243 R244 A245 K246 T247 V248 D249 L250 L251 A256 E257 I258 V259 I260 E261 G262 H263 V264 M265 P266 GLY ARG THR ALA VAL GLU GLY PRO MET GLY
GLU TYR ALA GLY TYR GLN PRO ARG HIS THR SER MET GLN P290 E291 Y292 V293 V294 D295 A296 I297 T298 Y299 R300 D301 D302 P303 I304 W305 P306 I378 R423 L433 L452 L456 M459 R462 T471 L483 L484 A485

4 Data and refinement statistics (i)

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 26.12 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (26.13-2.59) 99.8 (26.12-2.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 56.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, MG, UNL

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	0.53	0/3644	0.66	0/4977
1	B	0.54	0/3644	0.67	0/4977
1	C	0.47	0/3639	0.64	0/4971
1	D	0.45	0/3626	0.64	0/4954
All	All	0.50	0/14553	0.65	0/19879

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	3557	0	3555	2	0
1	B	3557	0	3555	4	0
1	C	3552	0	3549	5	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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: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
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:467:SER:H	1:C:471:THR:HG1	1.66	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 (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	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 (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	374/405 (92%)	373 (100%)	1 (0%)	92	98
1	B	374/405 (92%)	369 (99%)	5 (1%)	69	86
1	C	373/405 (92%)	371 (100%)	2 (0%)	88	96
1	D	372/405 (92%)	369 (99%)	3 (1%)	81	92
All	All	1493/1620 (92%)	1482 (99%)	11 (1%)	84	94

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

Mol	Chain	Res	Type
1	A	471	THR
1	B	25	GLU

Continued on next page...

Continued from previous page...

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	43	ASN
1	D	164	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	502	-	5,5,5	0.07	0	5,5,5	0.49	0
3	GOL	A	503	-	5,5,5	0.06	0	5,5,5	0.29	0
3	GOL	C	502	-	5,5,5	0.11	0	5,5,5	0.30	0
3	GOL	B	501	-	5,5,5	0.09	0	5,5,5	0.24	0
3	GOL	A	502	-	5,5,5	0.27	0	5,5,5	0.37	0
3	GOL	B	505	-	5,5,5	0.07	0	5,5,5	0.17	0
3	GOL	C	503	-	5,5,5	0.16	0	5,5,5	0.36	0
3	GOL	A	505	-	5,5,5	0.14	0	5,5,5	0.21	0
3	GOL	C	504	-	5,5,5	0.32	0	5,5,5	0.45	0
3	GOL	A	506	-	5,5,5	0.15	0	5,5,5	0.42	0
3	GOL	B	503	-	5,5,5	0.28	0	5,5,5	0.26	0
3	GOL	C	501	-	5,5,5	0.21	0	5,5,5	0.71	0
3	GOL	A	507	-	5,5,5	0.15	0	5,5,5	0.14	0
3	GOL	B	504	-	5,5,5	0.18	0	5,5,5	0.34	0
3	GOL	D	501	-	5,5,5	0.24	0	5,5,5	0.32	0
3	GOL	A	504	-	5,5,5	0.54	0	5,5,5	0.76	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	B	502	-	-	0/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	C	502	-	-	0/4/4/4	-
3	GOL	B	501	-	-	2/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	B	505	-	-	0/4/4/4	-
3	GOL	C	503	-	-	1/4/4/4	-
3	GOL	A	505	-	-	2/4/4/4	-
3	GOL	C	504	-	-	0/4/4/4	-
3	GOL	A	506	-	-	2/4/4/4	-
3	GOL	B	503	-	-	1/4/4/4	-
3	GOL	C	501	-	-	0/4/4/4	-
3	GOL	A	507	-	-	2/4/4/4	-
3	GOL	B	504	-	-	0/4/4/4	-
3	GOL	D	501	-	-	0/4/4/4	-
3	GOL	A	504	-	-	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	507	GOL	O1-C1-C2-C3
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	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	504	GOL	O1-C1-C2-C3
3	C	503	GOL	C1-C2-C3-O3
3	A	506	GOL	O2-C2-C3-O3
3	B	501	GOL	O2-C2-C3-O3
3	B	503	GOL	O2-C2-C3-O3

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	464/501 (92%)	0.24	26 (5%)	24	19	29, 47, 94, 118	0
1	B	464/501 (92%)	0.19	29 (6%)	20	15	29, 47, 85, 124	0
1	C	463/501 (92%)	0.82	84 (18%)	1	0	31, 71, 175, 228	0
1	D	461/501 (92%)	1.29	137 (29%)	0	0	28, 75, 208, 254	0
All	All	1852/2004 (92%)	0.63	276 (14%)	2	1	28, 55, 176, 254	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	173	ILE	12.0
1	D	128	ALA	9.7
1	D	194	LEU	9.6
1	D	183	ILE	9.0
1	C	189	GLY	8.1
1	D	174	ASP	7.8
1	A	184	PRO	7.6
1	D	265	MET	7.4
1	D	193	LYS	7.4
1	C	265	MET	7.4
1	D	114	ASP	7.2
1	C	194	LEU	7.1
1	C	196	ASP	6.9
1	D	126	ASP	6.9
1	D	293	VAL	6.7
1	D	115	SER	6.7
1	D	201	PRO	6.5
1	C	192	ARG	6.4
1	D	116	ALA	6.4
1	D	158	PRO	6.3
1	D	113	VAL	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	185	THR	6.1
1	D	190	GLN	6.0
1	B	193	LYS	5.9
1	D	111	VAL	5.9
1	D	184	PRO	5.9
1	D	195	TRP	5.8
1	B	185	THR	5.6
1	D	189	GLY	5.5
1	C	114	ASP	5.3
1	D	129	ASN	5.3
1	D	162	PHE	5.3
1	C	181	THR	5.2
1	D	177	ARG	5.2
1	D	198	LEU	5.1
1	D	133	PHE	5.0
1	D	249	ASP	4.9
1	B	184	PRO	4.8
1	D	297	ILE	4.8
1	A	185	THR	4.7
1	D	247	THR	4.7
1	D	459	MET	4.7
1	C	161	SER	4.7
1	D	196	ASP	4.7
1	D	60	CYS	4.5
1	D	299	TYR	4.5
1	D	123	LEU	4.5
1	A	266	PRO	4.5
1	C	247	THR	4.4
1	D	118	CYS	4.4
1	D	206	ILE	4.4
1	D	292	TYR	4.4
1	D	151	GLY	4.3
1	C	159	ASP	4.3
1	C	111	VAL	4.3
1	C	294	VAL	4.3
1	A	181	THR	4.2
1	C	88	VAL	4.2
1	C	123	LEU	4.2
1	C	177	ARG	4.2
1	D	171	MET	4.2
1	C	184	PRO	4.1
1	A	183	ILE	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	176	LYS	4.1
1	C	120	ASP	4.1
1	D	197	ASN	4.1
1	D	204	PHE	4.1
1	D	120	ASP	4.0
1	D	306	PRO	4.0
1	D	121	ASN	4.0
1	D	264	VAL	4.0
1	D	203	PRO	4.0
1	D	157	THR	3.8
1	D	161	SER	3.8
1	D	59	PHE	3.7
1	D	202	MET	3.7
1	C	193	LYS	3.7
1	D	263	HIS	3.7
1	D	192	ARG	3.7
1	D	122	VAL	3.6
1	A	460	ALA	3.6
1	D	208	GLN	3.6
1	D	179	THR	3.6
1	D	243	VAL	3.6
1	C	263	HIS	3.5
1	B	0	SER	3.5
1	D	191	ILE	3.5
1	D	165	TRP	3.5
1	C	292	TYR	3.4
1	C	183	ILE	3.4
1	D	127	ASP	3.4
1	C	109	ALA	3.4
1	D	209	GLY	3.4
1	D	301	ASP	3.4
1	D	124	LEU	3.4
1	C	158	PRO	3.4
1	C	246	LYS	3.4
1	D	119	GLN	3.3
1	D	304	ILE	3.3
1	D	150	TRP	3.3
1	D	305	TRP	3.3
1	D	248	VAL	3.2
1	D	303	PRO	3.2
1	B	214	ILE	3.2
1	D	181	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	197	ASN	3.2
1	C	249	ASP	3.2
1	C	155	VAL	3.2
1	C	1	MET	3.2
1	A	141	GLY	3.2
1	D	186	GLN	3.1
1	C	293	VAL	3.1
1	D	140	GLU	3.1
1	D	485	ALA	3.1
1	D	261	GLU	3.1
1	A	193	LYS	3.1
1	C	0	SER	3.1
1	C	197	ASN	3.1
1	D	160	GLY	3.1
1	D	300	ARG	3.1
1	C	139	HIS	3.1
1	C	115	SER	3.1
1	C	301	ASP	3.1
1	D	88	VAL	3.1
1	C	299	TYR	3.1
1	B	267	GLY	3.0
1	A	140	GLU	3.0
1	D	246	LYS	3.0
1	C	143	GLY	3.0
1	D	251	LEU	3.0
1	D	117	PRO	3.0
1	C	126	ASP	3.0
1	C	162	PHE	3.0
1	B	114	ASP	2.9
1	C	173	ILE	2.9
1	C	182	PHE	2.9
1	D	244	ARG	2.9
1	D	17	HIS	2.9
1	D	260	ILE	2.9
1	D	210	THR	2.9
1	D	224	ASP	2.9
1	C	296	ALA	2.9
1	D	295	ASP	2.9
1	C	295	ASP	2.8
1	D	125	GLY	2.8
1	A	153	ILE	2.8
1	C	172	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	154	ILE	2.8
1	D	135	ALA	2.8
1	B	63	LEU	2.8
1	C	464	ARG	2.8
1	D	225	GLY	2.8
1	D	141	GLY	2.8
1	C	186	GLN	2.8
1	C	156	SER	2.8
1	D	73	PRO	2.8
1	C	264	VAL	2.7
1	C	179	THR	2.7
1	D	156	SER	2.7
1	D	24	ASP	2.7
1	C	144	GLY	2.7
1	B	72	ILE	2.7
1	B	73	PRO	2.7
1	C	256	ALA	2.7
1	D	152	THR	2.7
1	D	187	HIS	2.7
1	C	171	MET	2.7
1	C	89	SER	2.7
1	C	140	GLU	2.7
1	C	132	ARG	2.6
1	D	44	ARG	2.6
1	A	478	GLN	2.6
1	D	132	ARG	2.6
1	D	112	VAL	2.6
1	C	116	ALA	2.6
1	B	154	ILE	2.6
1	B	209	GLY	2.6
1	C	153	ILE	2.6
1	A	367	PRO	2.6
1	C	297	ILE	2.6
1	D	205	ALA	2.6
1	D	298	THR	2.6
1	A	114	ASP	2.6
1	B	183	ILE	2.6
1	B	485	ALA	2.6
1	D	110	PRO	2.6
1	A	482	GLU	2.6
1	C	485	ALA	2.6
1	A	432	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	433	LEU	2.6
1	D	483	LEU	2.6
1	A	475	PRO	2.5
1	D	9	GLU	2.5
1	D	18	GLN	2.5
1	D	200	GLN	2.5
1	D	245	ALA	2.5
1	D	16	ALA	2.5
1	D	223	PRO	2.5
1	C	224	ASP	2.5
1	A	182	PHE	2.5
1	D	182	PHE	2.5
1	D	215	PRO	2.5
1	C	113	VAL	2.5
1	C	306	PRO	2.5
1	B	150	TRP	2.4
1	C	146	TYR	2.4
1	C	248	VAL	2.4
1	D	294	VAL	2.4
1	B	74	GLY	2.4
1	D	214	ILE	2.4
1	B	367	PRO	2.4
1	D	8	ARG	2.4
1	D	144	GLY	2.4
1	D	139	HIS	2.4
1	D	109	ALA	2.4
1	B	482	GLU	2.4
1	D	433	LEU	2.4
1	A	198	LEU	2.4
1	B	197	ASN	2.4
1	B	215	PRO	2.4
1	C	291	GLU	2.4
1	D	51	ASN	2.4
1	B	181	THR	2.4
1	D	89	SER	2.4
1	D	172	LYS	2.3
1	C	180	GLY	2.3
1	A	485	ALA	2.3
1	C	157	THR	2.3
1	D	163	THR	2.3
1	D	266	PRO	2.3
1	D	72	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	185	THR	2.3
1	C	259	VAL	2.3
1	C	254	ALA	2.3
1	D	166	ALA	2.3
1	A	152	THR	2.3
1	C	108	VAL	2.2
1	C	73	PRO	2.2
1	D	262	GLY	2.2
1	D	159	ASP	2.2
1	B	152	THR	2.2
1	D	71	THR	2.2
1	C	122	VAL	2.2
1	D	155	VAL	2.2
1	A	461	GLU	2.2
1	D	167	ILE	2.2
1	B	216	PHE	2.2
1	D	147	LEU	2.2
1	A	443	ARG	2.2
1	D	21	ARG	2.2
1	D	258	ILE	2.2
1	C	225	GLY	2.2
1	C	251	LEU	2.2
1	C	160	GLY	2.1
1	B	212	PRO	2.1
1	D	131	ASP	2.1
1	C	307	ILE	2.1
1	A	89	SER	2.1
1	D	378	ILE	2.1
1	C	188	LEU	2.1
1	C	250	LEU	2.1
1	B	306	PRO	2.1
1	C	337	LYS	2.1
1	C	207	VAL	2.1
1	B	478	GLN	2.1
1	C	141	GLY	2.1
1	A	196	ASP	2.0
1	C	245	ALA	2.0
1	D	256	ALA	2.0
1	A	169	ARG	2.0
1	C	201	PRO	2.0
1	D	291	GLU	2.0
1	C	262	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	206	ILE	2.0
1	B	66	PRO	2.0
1	B	475	PRO	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 monosaccharides 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	504	6/6	0.61	0.28	76,81,83,85	0
2	MG	D	503	1/1	0.62	0.41	73,73,73,73	0
2	MG	A	501	1/1	0.73	0.10	57,57,57,57	0
3	GOL	D	501	6/6	0.74	0.30	67,78,79,84	0
3	GOL	A	502	6/6	0.77	0.23	59,67,70,70	0
4	UNL	C	505	9/-	0.79	0.28	79,84,89,90	0
3	GOL	B	504	6/6	0.80	0.31	62,75,79,79	0
3	GOL	A	504	6/6	0.81	0.30	45,59,62,67	0
3	GOL	B	503	6/6	0.81	0.23	66,69,70,71	0
4	UNL	D	502	9/-	0.84	0.28	80,82,86,87	0
3	GOL	A	505	6/6	0.87	0.32	64,66,70,73	0
3	GOL	A	506	6/6	0.88	0.40	72,75,77,78	0
3	GOL	C	502	6/6	0.88	0.33	73,76,83,86	0
3	GOL	C	501	6/6	0.89	0.28	55,61,68,72	0
3	GOL	A	503	6/6	0.92	0.15	58,66,71,72	0
3	GOL	C	503	6/6	0.92	0.34	56,57,59,63	0
3	GOL	B	501	6/6	0.93	0.30	52,53,56,59	0
3	GOL	A	507	6/6	0.94	0.33	40,49,53,56	0
2	MG	B	506	1/1	0.94	0.04	59,59,59,59	0
3	GOL	B	502	6/6	0.94	0.16	54,54,55,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	505	6/6	0.95	0.32	66,71,73,75	0

6.5 Other polymers (i)

There are no such residues in this entry.