



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:54 PM UTC

PDB ID : 4QS5 / pdb_00004qs5
Title : CRYSTAL STRUCTURE of 5-CARBOXYVANILLATE DECARBOXYLASE
LIGW2 FROM NOVOSPHINGOBIUM AROMATICIVORANS DSM 12444
(TARGET EFI-505250) WITH BOUND MANGANESE AND 3-methoxy-4-hydroxy-5-nitrobenzoic acid, THE D314N MUTANT
Authors : Patskovsky, Y.; Vladimirova, A.; Toro, R.; Bhosle, R.; Hillerich, B.; Seidel, R.D.; Raushel, M.; Almo, S.C.
Deposited on : 2014-07-02
Resolution : 1.80 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)

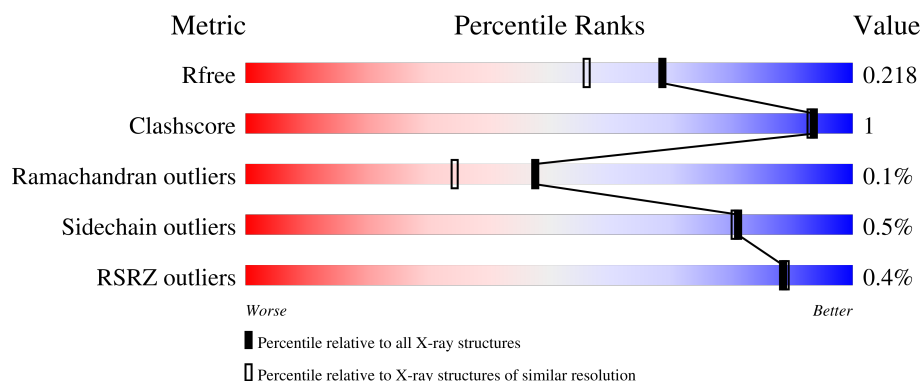
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

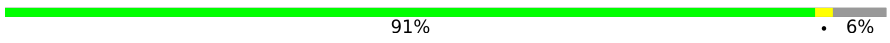
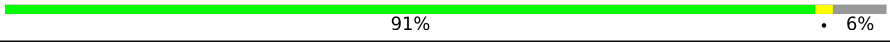
The reported resolution of this entry is 1.80 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	373	
1	B	373	
1	C	373	
1	D	373	

Validation Pipeline (wwPDB-VP) : 2.49

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
4	GOL	A	403	-	X	-	-
4	GOL	D	403	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12483 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 Ligw2 Decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	3	0
			2803	1781	481	522	19			
1	B	349	Total	C	N	O	S	0	2	0
			2794	1774	480	520	20			
1	C	348	Total	C	N	O	S	0	6	0
			2814	1787	481	525	21			
1	D	348	Total	C	N	O	S	0	3	0
			2792	1776	477	520	19			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q2GA79
A	-20	HIS	-	expression tag	UNP Q2GA79
A	-19	HIS	-	expression tag	UNP Q2GA79
A	-18	HIS	-	expression tag	UNP Q2GA79
A	-17	HIS	-	expression tag	UNP Q2GA79
A	-16	HIS	-	expression tag	UNP Q2GA79
A	-15	HIS	-	expression tag	UNP Q2GA79
A	-14	SER	-	expression tag	UNP Q2GA79
A	-13	SER	-	expression tag	UNP Q2GA79
A	-12	GLY	-	expression tag	UNP Q2GA79
A	-11	VAL	-	expression tag	UNP Q2GA79
A	-10	ASP	-	expression tag	UNP Q2GA79
A	-9	LEU	-	expression tag	UNP Q2GA79
A	-8	GLY	-	expression tag	UNP Q2GA79
A	-7	THR	-	expression tag	UNP Q2GA79
A	-6	GLU	-	expression tag	UNP Q2GA79
A	-5	ASN	-	expression tag	UNP Q2GA79
A	-4	LEU	-	expression tag	UNP Q2GA79
A	-3	TYR	-	expression tag	UNP Q2GA79
A	-2	PHE	-	expression tag	UNP Q2GA79
A	-1	GLN	-	expression tag	UNP Q2GA79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q2GA79
A	314	ASN	ASP	engineered mutation	UNP Q2GA79
B	-21	MET	-	expression tag	UNP Q2GA79
B	-20	HIS	-	expression tag	UNP Q2GA79
B	-19	HIS	-	expression tag	UNP Q2GA79
B	-18	HIS	-	expression tag	UNP Q2GA79
B	-17	HIS	-	expression tag	UNP Q2GA79
B	-16	HIS	-	expression tag	UNP Q2GA79
B	-15	HIS	-	expression tag	UNP Q2GA79
B	-14	SER	-	expression tag	UNP Q2GA79
B	-13	SER	-	expression tag	UNP Q2GA79
B	-12	GLY	-	expression tag	UNP Q2GA79
B	-11	VAL	-	expression tag	UNP Q2GA79
B	-10	ASP	-	expression tag	UNP Q2GA79
B	-9	LEU	-	expression tag	UNP Q2GA79
B	-8	GLY	-	expression tag	UNP Q2GA79
B	-7	THR	-	expression tag	UNP Q2GA79
B	-6	GLU	-	expression tag	UNP Q2GA79
B	-5	ASN	-	expression tag	UNP Q2GA79
B	-4	LEU	-	expression tag	UNP Q2GA79
B	-3	TYR	-	expression tag	UNP Q2GA79
B	-2	PHE	-	expression tag	UNP Q2GA79
B	-1	GLN	-	expression tag	UNP Q2GA79
B	0	SER	-	expression tag	UNP Q2GA79
B	314	ASN	ASP	engineered mutation	UNP Q2GA79
C	-21	MET	-	expression tag	UNP Q2GA79
C	-20	HIS	-	expression tag	UNP Q2GA79
C	-19	HIS	-	expression tag	UNP Q2GA79
C	-18	HIS	-	expression tag	UNP Q2GA79
C	-17	HIS	-	expression tag	UNP Q2GA79
C	-16	HIS	-	expression tag	UNP Q2GA79
C	-15	HIS	-	expression tag	UNP Q2GA79
C	-14	SER	-	expression tag	UNP Q2GA79
C	-13	SER	-	expression tag	UNP Q2GA79
C	-12	GLY	-	expression tag	UNP Q2GA79
C	-11	VAL	-	expression tag	UNP Q2GA79
C	-10	ASP	-	expression tag	UNP Q2GA79
C	-9	LEU	-	expression tag	UNP Q2GA79
C	-8	GLY	-	expression tag	UNP Q2GA79
C	-7	THR	-	expression tag	UNP Q2GA79
C	-6	GLU	-	expression tag	UNP Q2GA79
C	-5	ASN	-	expression tag	UNP Q2GA79

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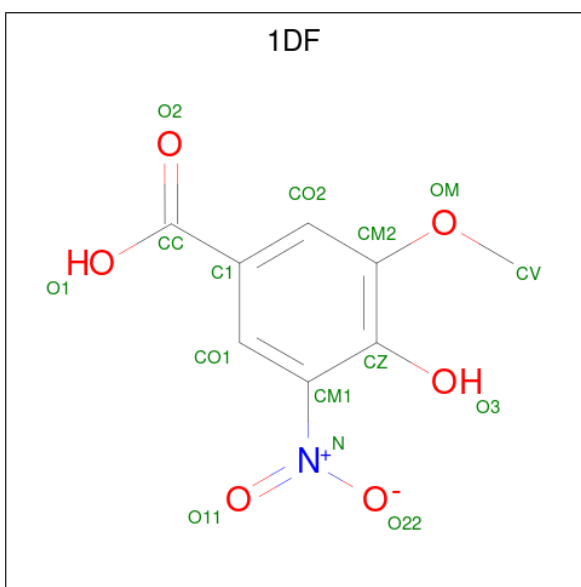
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	LEU	-	expression tag	UNP Q2GA79
C	-3	TYR	-	expression tag	UNP Q2GA79
C	-2	PHE	-	expression tag	UNP Q2GA79
C	-1	GLN	-	expression tag	UNP Q2GA79
C	0	SER	-	expression tag	UNP Q2GA79
C	314	ASN	ASP	engineered mutation	UNP Q2GA79
D	-21	MET	-	expression tag	UNP Q2GA79
D	-20	HIS	-	expression tag	UNP Q2GA79
D	-19	HIS	-	expression tag	UNP Q2GA79
D	-18	HIS	-	expression tag	UNP Q2GA79
D	-17	HIS	-	expression tag	UNP Q2GA79
D	-16	HIS	-	expression tag	UNP Q2GA79
D	-15	HIS	-	expression tag	UNP Q2GA79
D	-14	SER	-	expression tag	UNP Q2GA79
D	-13	SER	-	expression tag	UNP Q2GA79
D	-12	GLY	-	expression tag	UNP Q2GA79
D	-11	VAL	-	expression tag	UNP Q2GA79
D	-10	ASP	-	expression tag	UNP Q2GA79
D	-9	LEU	-	expression tag	UNP Q2GA79
D	-8	GLY	-	expression tag	UNP Q2GA79
D	-7	THR	-	expression tag	UNP Q2GA79
D	-6	GLU	-	expression tag	UNP Q2GA79
D	-5	ASN	-	expression tag	UNP Q2GA79
D	-4	LEU	-	expression tag	UNP Q2GA79
D	-3	TYR	-	expression tag	UNP Q2GA79
D	-2	PHE	-	expression tag	UNP Q2GA79
D	-1	GLN	-	expression tag	UNP Q2GA79
D	0	SER	-	expression tag	UNP Q2GA79
D	314	ASN	ASP	engineered mutation	UNP Q2GA79

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

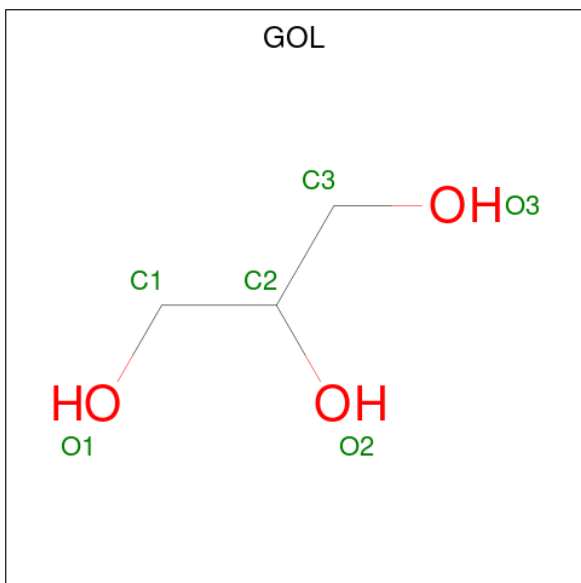
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

- Molecule 3 is 4-hydroxy-3-methoxy-5-nitrobenzoic acid (CCD ID: 1DF) (formula: C₈H₇NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		
3	C	1	Total	C	N	O	0	0
			15	8	1	6		
3	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

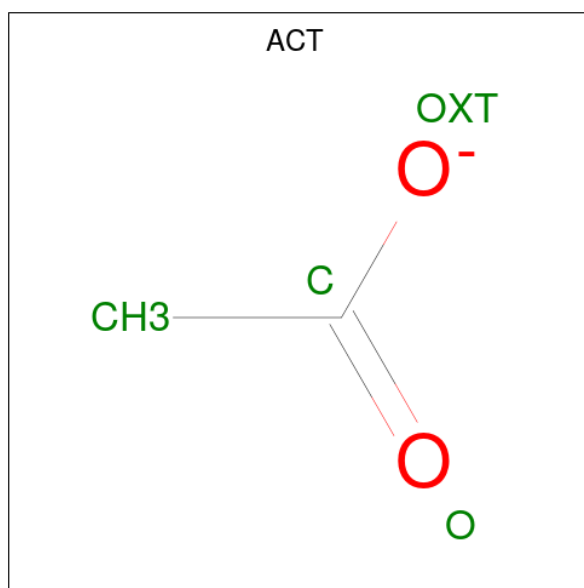


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

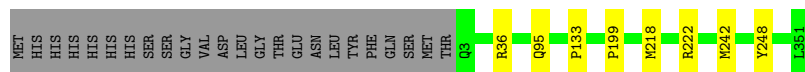
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	268	Total	O	0	1
			269	269		
7	B	284	Total	O	0	0
			284	284		
7	C	313	Total	O	0	1
			314	314		
7	D	290	Total	O	0	1
			291	291		

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.

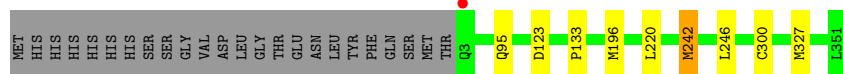
- Molecule 1: Ligw2 Decarboxylase

Chain A:  91% 6%

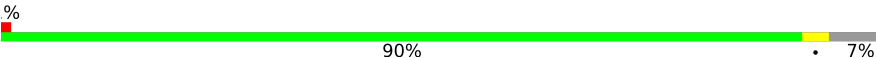


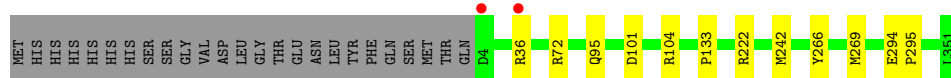
- Molecule 1: Ligw2 Decarboxylase

Chain B:  91% 6%

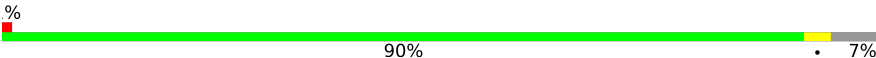


- Molecule 1: Ligw2 Decarboxylase

Chain C:  90% 7%



- Molecule 1: Ligw2 Decarboxylase

Chain D:  90% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.16Å 60.59Å 123.47Å 90.00° 112.84° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.80) 99.8 (50.00-1.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.156 , 0.210 (Not available) , 0.218	Depositor DCC
R_{free} test set	3722 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12483	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.0937e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, ACT, MN, 1DF, CL

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	0.72	0/2874	0.83	0/3881
1	B	0.74	0/2859	0.83	0/3862
1	C	0.76	0/2888	0.86	0/3901
1	D	0.76	1/2863 (0.0%)	0.87	0/3866
All	All	0.74	1/11484 (0.0%)	0.85	0/15510

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	202	GLU	C-O	-5.01	1.18	1.24

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	2803	0	2768	9	0
1	B	2794	0	2749	7	0
1	C	2814	0	2774	10	0
1	D	2792	0	2760	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	15	0	5	0	0
3	B	15	0	5	0	0
3	C	15	0	5	0	0
3	D	15	0	5	0	0
4	A	6	0	7	0	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
4	D	18	0	24	2	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
6	A	4	0	3	0	0
6	C	4	0	3	0	0
7	A	269	0	0	0	0
7	B	284	0	0	0	0
7	C	314	0	0	0	0
7	D	291	0	0	0	0
All	All	12483	0	11140	32	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 (32) 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:C:36[B]:ARG:CG	1:C:36[B]:ARG:HH11	1.70	1.05
1:C:36[B]:ARG:HH11	1:C:36[B]:ARG:HG3	1.18	1.01
1:A:36[B]:ARG:HH11	1:A:36[B]:ARG:CG	1.76	0.98
1:C:36[B]:ARG:HG3	1:C:36[B]:ARG:NH1	1.86	0.82
1:A:36[B]:ARG:HH11	1:A:36[B]:ARG:HG3	1.42	0.82
1:A:36[B]:ARG:HH11	1:A:36[B]:ARG:HG2	1.54	0.71
1:A:36[B]:ARG:HG3	1:A:36[B]:ARG:NH1	2.09	0.66
1:C:266:TYR:CD2	1:C:269[B]:MET:HE2	2.33	0.63
1:C:36[B]:ARG:CG	1:C:36[B]:ARG:NH1	2.41	0.61
1:C:36[B]:ARG:HH11	1:C:36[B]:ARG:HG2	1.64	0.60
1:D:162:GLN:HA	4:D:403:GOL:H12	1.85	0.58
1:B:220:LEU:HD23	1:B:246:LEU:HD12	1.89	0.54
1:A:36[B]:ARG:CG	1:A:36[B]:ARG:NH1	2.48	0.54
1:D:220:LEU:HD23	1:D:246:LEU:HD12	1.92	0.52
1:C:222:ARG:NH2	1:D:202:GLU:OE2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:PRO:HG2	1:B:196:MET:HG3	1.93	0.49
1:B:95:GLN:HG2	1:B:133:PRO:HD2	1.94	0.49
1:A:248:TYR:OH	1:B:300[B]:CYS:SG	2.71	0.47
1:C:95:GLN:HG2	1:C:133:PRO:HD2	1.98	0.46
1:D:202:GLU:O	1:D:202:GLU:HG2	2.16	0.46
1:B:123:ASP:HB2	5:B:405:CL:CL	2.54	0.44
1:A:218:MET:O	1:A:222:ARG:HG2	2.17	0.44
1:C:294[A]:GLU:HB3	1:C:295:PRO:HD3	1.98	0.44
1:D:242:MET:HE3	1:D:242:MET:HA	2.00	0.43
1:A:95:GLN:HG2	1:A:133:PRO:HD2	2.00	0.43
1:B:327:MET:HA	1:B:327:MET:HE2	2.01	0.42
1:D:95:GLN:HG2	1:D:133:PRO:HD2	2.01	0.42
1:D:293:TRP:HE1	4:D:404:GOL:C3	2.32	0.42
1:D:332:MET:HG2	1:D:336:THR:HB	2.01	0.41
1:D:327:MET:HA	1:D:327:MET:HE2	2.03	0.41
1:C:101[B]:ASP:OD1	1:C:104:ARG:NH2	2.54	0.40
1:B:242:MET:HA	1:B:242:MET:HE3	2.02	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	350/373 (94%)	340 (97%)	10 (3%)	0	100	100
1	B	349/373 (94%)	338 (97%)	11 (3%)	0	100	100
1	C	352/373 (94%)	341 (97%)	11 (3%)	0	100	100
1	D	349/373 (94%)	338 (97%)	10 (3%)	1 (0%)	36	25
All	All	1400/1492 (94%)	1357 (97%)	42 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	210	PHE

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	293/312 (94%)	292 (100%)	1 (0%)	86	86
1	B	291/312 (93%)	290 (100%)	1 (0%)	86	86
1	C	295/312 (95%)	293 (99%)	2 (1%)	76	73
1	D	292/312 (94%)	290 (99%)	2 (1%)	76	73
All	All	1171/1248 (94%)	1165 (100%)	6 (0%)	81	80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	MET
1	B	242	MET
1	C	72	ARG
1	C	242	MET
1	D	119	GLN
1	D	302	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	156	GLN
1	A	158	ASN
1	A	258	GLN
1	B	156	GLN
1	B	158	ASN
1	B	258	GLN
1	C	98	HIS
1	C	156	GLN
1	C	158	ASN

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Mol	Chain	Res	Type
1	C	302	GLN
1	D	156	GLN
1	D	158	ASN
1	D	264	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	1DF	D	402	2	15,15,15	0.97	1 (6%)	16,21,21	1.73	3 (18%)
4	GOL	D	405	-	5,5,5	0.34	0	5,5,5	0.39	0
4	GOL	C	403	-	5,5,5	0.49	0	5,5,5	0.73	0
3	1DF	A	402	2	15,15,15	2.43	1 (6%)	16,21,21	2.20	6 (37%)
3	1DF	B	402	2	15,15,15	1.57	1 (6%)	16,21,21	1.96	4 (25%)
4	GOL	C	404	-	5,5,5	0.31	0	5,5,5	0.49	0
6	ACT	C	405	-	3,3,3	0.69	0	3,3,3	1.34	0
4	GOL	D	403	-	5,5,5	0.80	0	5,5,5	1.73	2 (40%)
4	GOL	B	404	-	5,5,5	0.33	0	5,5,5	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	A	405	-	3,3,3	0.80	0	3,3,3	0.82	0
4	GOL	A	403	-	5,5,5	0.83	0	5,5,5	1.80	3 (60%)
4	GOL	B	403	-	5,5,5	0.25	0	5,5,5	0.19	0
3	1DF	C	402	2	15,15,15	1.75	2 (13%)	16,21,21	1.89	5 (31%)
4	GOL	D	404	-	5,5,5	0.42	0	5,5,5	1.41	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	1DF	D	402	2	-	0/8/10/10	0/1/1/1
4	GOL	D	405	-	-	3/4/4/4	-
4	GOL	C	403	-	-	4/4/4/4	-
3	1DF	A	402	2	-	2/8/10/10	0/1/1/1
3	1DF	B	402	2	-	0/8/10/10	0/1/1/1
4	GOL	C	404	-	-	2/4/4/4	-
4	GOL	D	403	-	-	4/4/4/4	-
4	GOL	B	404	-	-	0/4/4/4	-
4	GOL	A	403	-	-	4/4/4/4	-
4	GOL	B	403	-	-	0/4/4/4	-
3	1DF	C	402	2	-	0/8/10/10	0/1/1/1
4	GOL	D	404	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	1DF	CM1-N	8.82	1.61	1.45
3	C	402	1DF	CM1-N	5.76	1.56	1.45
3	B	402	1DF	CM1-N	5.34	1.55	1.45
3	C	402	1DF	CM2-CZ	-2.38	1.37	1.40
3	D	402	1DF	CM2-CZ	-2.04	1.37	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	1DF	OM-CM2-CZ	4.78	119.53	114.53
3	A	402	1DF	OM-CM2-CZ	4.63	119.37	114.53
3	C	402	1DF	OM-CM2-CZ	4.06	118.78	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	1DF	CV-OM-CM2	4.02	123.40	117.51
3	A	402	1DF	O11-N-CM1	3.99	125.85	119.03
3	D	402	1DF	OM-CM2-CZ	3.83	118.53	114.53
3	C	402	1DF	O11-N-CM1	3.62	125.22	119.03
3	B	402	1DF	O11-N-CM1	3.58	125.16	119.03
3	C	402	1DF	CV-OM-CM2	3.24	122.27	117.51
3	D	402	1DF	O11-N-CM1	3.18	124.47	119.03
3	B	402	1DF	CV-OM-CM2	3.15	122.13	117.51
4	D	403	GOL	O1-C1-C2	-2.85	97.54	110.38
3	D	402	1DF	CV-OM-CM2	2.60	121.32	117.51
3	A	402	1DF	O3-CZ-CM1	-2.34	117.78	120.89
4	A	403	GOL	O2-C2-C1	2.22	118.36	109.18
3	A	402	1DF	CO1-CM1-CZ	-2.18	119.32	121.54
3	A	402	1DF	O1-CC-C1	2.13	120.31	114.84
4	D	403	GOL	O2-C2-C3	2.12	117.96	109.18
4	A	403	GOL	C3-C2-C1	-2.07	104.19	111.80
4	A	403	GOL	O3-C3-C2	-2.06	101.11	110.38
3	C	402	1DF	O1-CC-C1	2.06	120.12	114.84
3	B	402	1DF	O1-CC-O2	-2.03	118.99	123.35
3	C	402	1DF	CO1-CM1-CZ	-2.02	119.49	121.54

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	GOL	O1-C1-C2-C3
4	A	403	GOL	C1-C2-C3-O3
4	A	403	GOL	O2-C2-C3-O3
4	C	403	GOL	O1-C1-C2-C3
4	C	403	GOL	C1-C2-C3-O3
4	D	403	GOL	O1-C1-C2-O2
4	D	403	GOL	O1-C1-C2-C3
4	D	403	GOL	C1-C2-C3-O3
4	A	403	GOL	O1-C1-C2-O2
4	C	404	GOL	C1-C2-C3-O3
4	D	405	GOL	C1-C2-C3-O3
4	D	403	GOL	O2-C2-C3-O3
4	C	403	GOL	O1-C1-C2-O2
4	C	403	GOL	O2-C2-C3-O3
4	D	405	GOL	O1-C1-C2-O2
3	A	402	1DF	CO2-C1-CC-O1
4	D	405	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	404	GOL	O2-C2-C3-O3
3	A	402	1DF	CO2-C1-CC-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	403	GOL	1	0
4	D	404	GOL	1	0

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	349/373 (93%)	-0.39	0	100 100	12, 21, 42, 90	3 (0%)
1	B	349/373 (93%)	-0.42	1 (0%)	90 90	9, 21, 43, 69	2 (0%)
1	C	348/373 (93%)	-0.44	2 (0%)	85 86	10, 19, 38, 74	6 (1%)
1	D	348/373 (93%)	-0.48	2 (0%)	85 86	11, 20, 44, 71	3 (0%)
All	All	1394/1492 (93%)	-0.43	5 (0%)	88 89	9, 20, 43, 90	14 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	GLN	4.4
1	C	36[A]	ARG	2.7
1	C	4	ASP	2.3
1	D	302	GLN	2.2
1	D	137	GLU	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	GOL	C	404	6/6	0.79	0.18	40,49,76,77	0
4	GOL	D	404	6/6	0.81	0.19	32,57,73,99	0
4	GOL	D	405	6/6	0.82	0.18	28,52,59,64	0
4	GOL	B	404	6/6	0.83	0.17	27,38,67,117	0
4	GOL	A	403	6/6	0.84	0.17	24,58,70,74	0
4	GOL	C	403	6/6	0.87	0.12	19,30,52,62	0
4	GOL	B	403	6/6	0.88	0.13	27,42,46,52	0
4	GOL	D	403	6/6	0.90	0.12	21,29,53,58	0
5	CL	B	405	1/1	0.91	0.11	49,49,49,49	0
5	CL	A	404	1/1	0.95	0.13	44,44,44,44	0
3	1DF	A	402	15/15	0.95	0.07	17,24,53,81	0
6	ACT	C	405	4/4	0.95	0.13	20,38,39,64	0
3	1DF	D	402	15/15	0.96	0.07	15,19,36,57	0
3	1DF	B	402	15/15	0.96	0.07	17,21,39,55	0
3	1DF	C	402	15/15	0.96	0.07	14,23,54,65	0
6	ACT	A	405	4/4	0.97	0.08	18,25,36,74	0
2	MN	A	401	1/1	0.99	0.03	23,23,23,23	0
2	MN	B	401	1/1	0.99	0.03	20,20,20,20	0
2	MN	C	401	1/1	1.00	0.03	22,22,22,22	0
2	MN	D	401	1/1	1.00	0.04	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.