



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 11:07 AM UTC

PDB ID : 6LIV / pdb_00006liv
Title : Crystal structure of Tyrosine decarboxylase in complex with PLP
Authors : Wang, H.; Yu, J.; Yao, M.
Deposited on : 2019-12-13
Resolution : 2.31 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

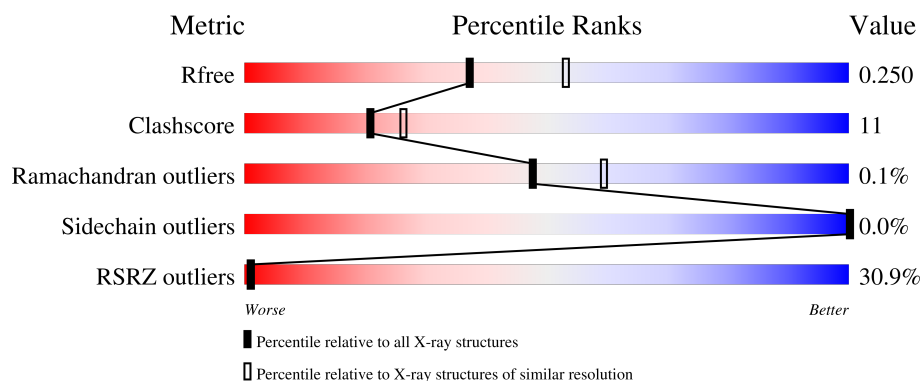
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	531	4% 80% 11% 9%
1	B	531	3% 81% 10% 9%
1	C	531	5% 79% 12% 9%
1	D	531	3% 81% 9% 9%
1	E	531	80% 56% 34% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	531	72% 52% 37% 10%

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	GOL	C	601	-	-	X	-
2	GOL	D	601	-	-	X	-
2	GOL	D	602	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23982 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 Tyrosine/DOPA decarboxylase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	P	S	0	0	0
			3840	2464	643	708	1	24			
1	B	483	Total	C	N	O	P	S	0	0	0
			3823	2454	639	705	1	24			
1	C	485	Total	C	N	O	P	S	0	0	0
			3840	2464	643	708	1	24			
1	D	483	Total	C	N	O	P	S	0	0	0
			3823	2454	639	705	1	24			
1	E	479	Total	C	N	O	P	S	0	0	0
			3802	2442	635	700	1	24			
1	F	477	Total	C	N	O	P	S	0	0	0
			3782	2429	633	695	1	24			

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



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

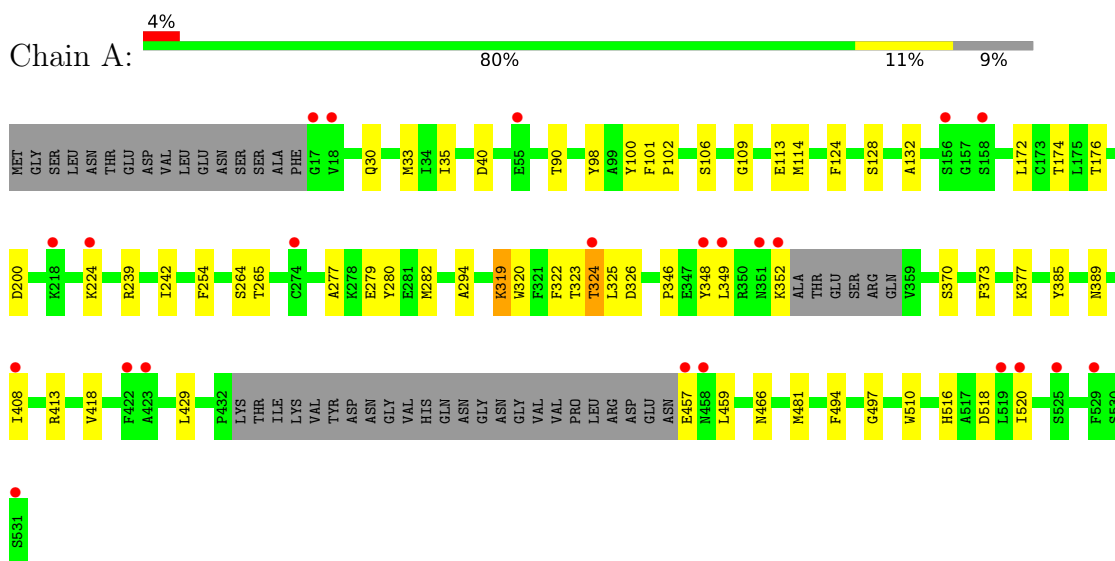
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	213	Total O 213 213	0	0
3	B	262	Total O 262 262	0	0
3	C	204	Total O 204 204	0	0
3	D	269	Total O 269 269	0	0
3	E	29	Total O 29 29	0	0
3	F	41	Total O 41 41	0	0

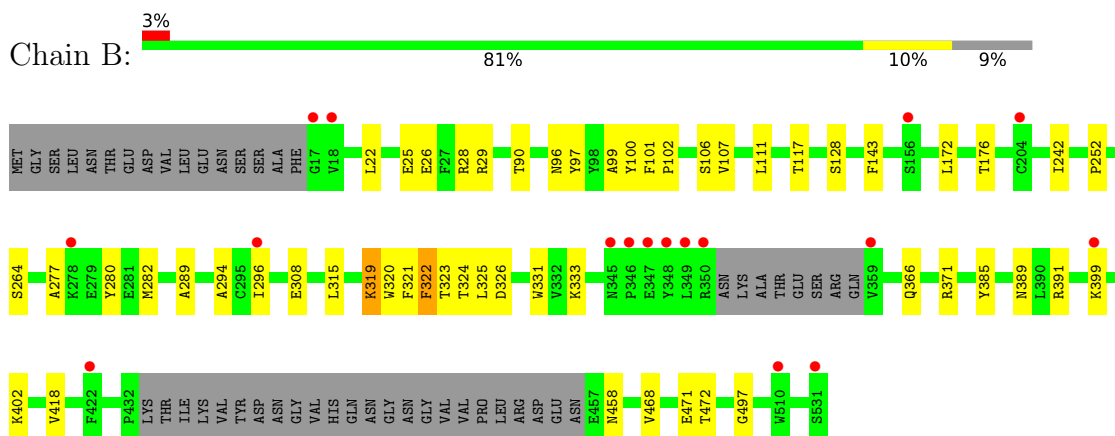
3 Residue-property plots [i](#)

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.

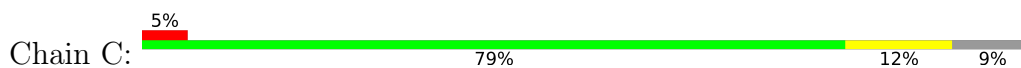
• Molecule 1: Tyrosine/DOPA decarboxylase 2

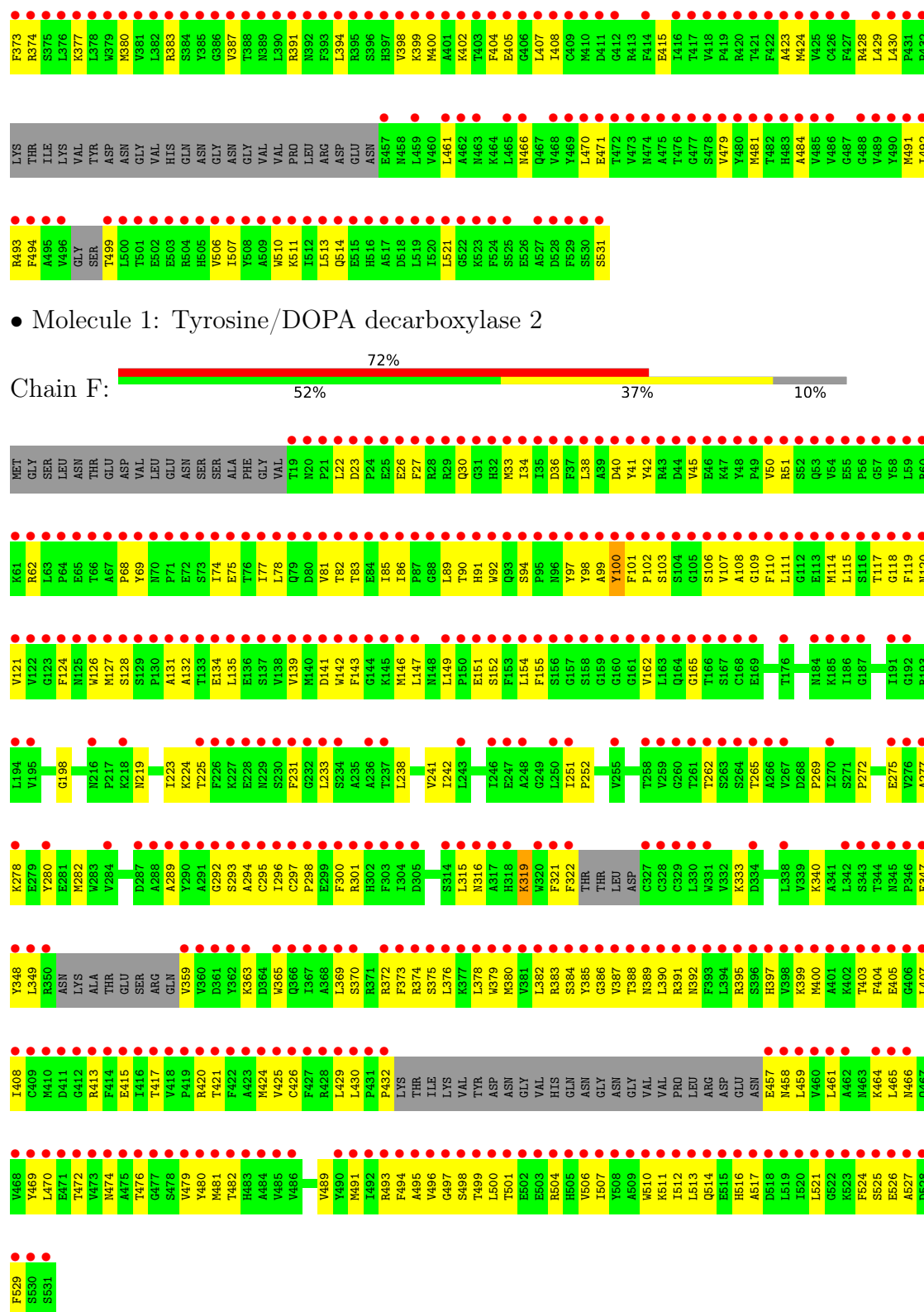


• Molecule 1: Tyrosine/DOPA decarboxylase 2



• Molecule 1: Tyrosine/DOPA decarboxylase 2





● Molecule 1: Tyrosine/DOPA decarboxylase 2

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	117.91Å 180.41Å 218.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 2.31 49.84 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.84-2.31) 99.6 (49.84-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.227 , 0.250 0.227 , 0.250	Depositor DCC
R_{free} test set	10120 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23982	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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 36.97 % 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 4.6058e-04. 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: LLP, 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	0.27	3/3909 (0.1%)	0.33	0/5307
1	B	0.36	4/3892 (0.1%)	0.40	4/5285 (0.1%)
1	C	0.34	4/3909 (0.1%)	0.36	1/5307 (0.0%)
1	D	0.20	0/3892	0.33	0/5285
1	E	0.25	1/3870 (0.0%)	0.40	0/5254
1	F	0.28	0/3850	0.50	2/5225 (0.0%)
All	All	0.29	12/23322 (0.1%)	0.39	7/31663 (0.0%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	471	GLU	C-O	-8.10	1.14	1.24
1	C	100	TYR	C-O	-7.58	1.14	1.24
1	B	100	TYR	C-O	-6.95	1.15	1.24
1	A	100	TYR	C-O	-6.89	1.15	1.24
1	C	101	PHE	C-O	-6.32	1.17	1.24

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	PHE	N-CA-C	8.54	123.38	113.38
1	B	321	PHE	N-CA-C	7.57	122.01	111.56
1	B	323	THR	N-CA-C	6.92	119.84	111.82
1	C	263	SER	N-CA-C	6.49	118.14	111.14
1	B	324	THR	N-CA-CB	5.42	119.64	110.49

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	3840	0	3783	42	0
1	B	3823	0	3764	35	0
1	C	3840	0	3783	52	0
1	D	3823	0	3764	43	0
1	E	3802	0	3743	156	0
1	F	3782	0	3721	227	0
2	A	6	0	8	3	0
2	B	18	0	24	3	0
2	C	18	0	24	10	0
2	D	12	0	16	7	0
3	A	213	0	0	2	0
3	B	262	0	0	1	0
3	C	204	0	0	3	0
3	D	269	0	0	3	0
3	E	29	0	0	1	0
3	F	41	0	0	3	0
All	All	23982	0	22630	506	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 11.

The worst 5 of 506 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:319:LLP:H4'1	2:C:601:GOL:H11	1.23	1.14
1:C:203:HIS:NE2	2:C:601:GOL:H12	1.67	1.08
1:C:203:HIS:HE2	2:C:601:GOL:H12	1.00	1.07
1:F:385:TYR:HB3	1:F:390:LEU:HD21	1.44	0.99
1:F:131:ALA:O	1:F:135:LEU:HD12	1.61	0.98

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	478/531 (90%)	466 (98%)	11 (2%)	1 (0%)	43	53
1	B	476/531 (90%)	465 (98%)	11 (2%)	0	100	100
1	C	478/531 (90%)	465 (97%)	13 (3%)	0	100	100
1	D	476/531 (90%)	465 (98%)	11 (2%)	0	100	100
1	E	470/531 (88%)	454 (97%)	15 (3%)	1 (0%)	43	53
1	F	468/531 (88%)	443 (95%)	25 (5%)	0	100	100
All	All	2846/3186 (89%)	2758 (97%)	86 (3%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	100	TYR
1	A	324	THR

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	415/455 (91%)	415 (100%)	0	100	100
1	B	413/455 (91%)	413 (100%)	0	100	100
1	C	415/455 (91%)	415 (100%)	0	100	100
1	D	413/455 (91%)	412 (100%)	1 (0%)	87	94
1	E	411/455 (90%)	411 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	408/455 (90%)	408 (100%)	0	100	100
All	All	2475/2730 (91%)	2474 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	262	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	302	HIS
1	E	392	ASN
1	F	514	GLN
1	F	30	GLN
1	F	120	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	D	319	1	23,24,25	2.50	6 (26%)	25,32,34	1.31	4 (16%)
1	LLP	E	319	1	23,24,25	2.48	6 (26%)	25,32,34	1.40	3 (12%)
1	LLP	A	319	1	23,24,25	2.48	6 (26%)	25,32,34	1.32	4 (16%)
1	LLP	C	319	1	23,24,25	2.49	6 (26%)	25,32,34	1.34	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	F	319	1	23,24,25	2.48	6 (26%)	25,32,34	1.39	4 (16%)
1	LLP	B	319	1	23,24,25	2.49	6 (26%)	25,32,34	1.30	4 (16%)

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
1	LLP	D	319	1	-	2/16/17/19	0/1/1/1
1	LLP	E	319	1	-	6/16/17/19	0/1/1/1
1	LLP	A	319	1	-	2/16/17/19	0/1/1/1
1	LLP	C	319	1	-	2/16/17/19	0/1/1/1
1	LLP	F	319	1	-	5/16/17/19	0/1/1/1
1	LLP	B	319	1	-	2/16/17/19	0/1/1/1

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	319	LLP	C4-C4'	7.23	1.62	1.46
1	D	319	LLP	C4-C4'	7.20	1.62	1.46
1	B	319	LLP	C4-C4'	7.16	1.61	1.46
1	F	319	LLP	C4-C4'	7.15	1.61	1.46
1	A	319	LLP	C4-C4'	7.14	1.61	1.46

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	319	LLP	C4-C4'-NZ	-3.69	107.01	124.04
1	F	319	LLP	C4-C4'-NZ	-3.45	108.11	124.04
1	B	319	LLP	C4-C4'-NZ	-3.44	108.15	124.04
1	C	319	LLP	C4-C4'-NZ	-3.44	108.15	124.04
1	A	319	LLP	C4-C4'-NZ	-3.41	108.29	124.04

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	319	LLP	C-CA-CB-CG
1	B	319	LLP	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	C	319	LLP	C-CA-CB-CG
1	D	319	LLP	C-CA-CB-CG
1	E	319	LLP	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	319	LLP	4	0
1	E	319	LLP	1	0
1	A	319	LLP	3	0
1	C	319	LLP	2	0
1	F	319	LLP	1	0
1	B	319	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	D	602	-	5,5,5	0.44	0	5,5,5	0.68	0
2	GOL	B	602	-	5,5,5	0.32	0	5,5,5	0.67	0
2	GOL	B	603	-	5,5,5	0.73	0	5,5,5	1.10	0
2	GOL	A	601	-	5,5,5	0.27	0	5,5,5	1.05	0
2	GOL	C	601	-	5,5,5	0.15	0	5,5,5	0.75	0
2	GOL	C	603	-	5,5,5	0.63	0	5,5,5	1.24	1 (20%)
2	GOL	B	601	-	5,5,5	0.44	0	5,5,5	0.73	0
2	GOL	D	601	-	5,5,5	0.61	0	5,5,5	0.46	0
2	GOL	C	602	-	5,5,5	0.25	0	5,5,5	0.59	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	D	602	-	-	2/4/4/4	-
2	GOL	B	602	-	-	0/4/4/4	-
2	GOL	B	603	-	-	2/4/4/4	-
2	GOL	A	601	-	-	4/4/4/4	-
2	GOL	C	601	-	-	4/4/4/4	-
2	GOL	C	603	-	-	2/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	D	601	-	-	4/4/4/4	-
2	GOL	C	602	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	GOL	O3-C3-C2	2.23	120.42	110.38

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-C3
2	B	601	GOL	O1-C1-C2-C3
2	C	601	GOL	C1-C2-C3-O3
2	C	602	GOL	C1-C2-C3-O3
2	C	603	GOL	O1-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	602	GOL	4	0
2	A	601	GOL	3	0
2	C	601	GOL	6	0
2	C	603	GOL	2	0
2	B	601	GOL	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	GOL	4	0
2	C	602	GOL	2	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	484/531 (91%)	0.32	23 (4%) 35 38	21, 30, 47, 74	0
1	B	482/531 (90%)	0.18	17 (3%) 47 50	21, 28, 43, 86	0
1	C	484/531 (91%)	0.36	29 (5%) 27 30	20, 30, 51, 83	0
1	D	482/531 (90%)	0.21	16 (3%) 49 52	20, 28, 43, 77	0
1	E	478/531 (90%)	3.99	426 (89%) 0 0	52, 76, 91, 101	0
1	F	476/531 (89%)	3.99	382 (80%) 0 0	43, 74, 96, 104	0
All	All	2886/3186 (90%)	1.50	893 (30%) 1 1	20, 33, 89, 104	0

The worst 5 of 893 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	387	VAL	10.7
1	E	22	LEU	10.4
1	F	382	LEU	10.0
1	F	74	ILE	9.7
1	E	500	LEU	9.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	E	319	24/25	0.80	0.20	60,68,78,81	0
1	LLP	F	319	24/25	0.85	0.20	44,56,72,76	0
1	LLP	C	319	24/25	0.95	0.08	21,28,31,34	0
1	LLP	D	319	24/25	0.95	0.08	19,23,28,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	A	319	24/25	0.96	0.07	19,24,30,31	0
1	LLP	B	319	24/25	0.96	0.08	19,25,29,30	0

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	601	6/6	0.76	0.18	26,35,37,38	6
2	GOL	C	602	6/6	0.76	0.20	29,38,40,43	6
2	GOL	B	603	6/6	0.80	0.18	18,26,28,31	6
2	GOL	B	601	6/6	0.82	0.17	24,30,32,35	6
2	GOL	C	603	6/6	0.84	0.17	28,35,38,39	6
2	GOL	B	602	6/6	0.85	0.15	29,31,32,33	6
2	GOL	D	601	6/6	0.86	0.15	23,28,34,34	6
2	GOL	A	601	6/6	0.88	0.14	27,31,32,35	6
2	GOL	D	602	6/6	0.88	0.14	30,32,32,36	6

6.5 Other polymers [i](#)

There are no such residues in this entry.