



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 12:12 PM EDT

PDB ID : 6Y4Y
Title : The crystal structure of human MACROD2 in space group P41212
Authors : Wazir, S.; Maksimainen, M.M.; Lehtio, L.
Deposited on : 2020-02-24
Resolution : 1.75 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

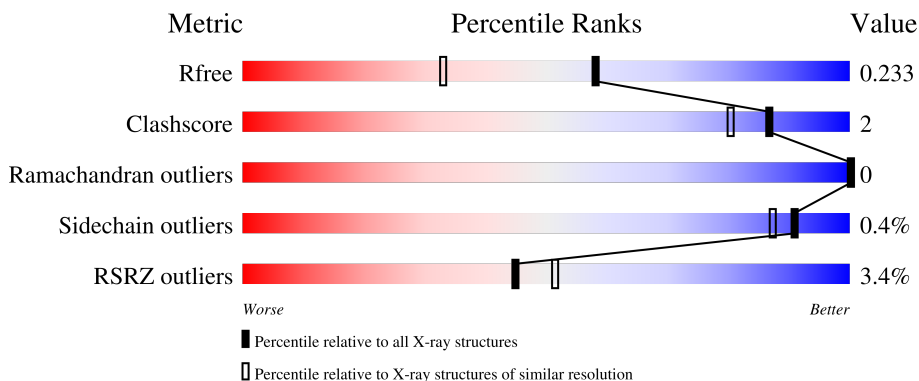
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	366	<div> <div> <div></div> <div>57%</div> <div>42%</div> </div> </div>
1	B	366	<div> <div> <div></div> <div>56%</div> <div>41%</div> </div> </div>
1	C	366	<div> <div> <div></div> <div>54%</div> <div>6%</div> <div>40%</div> </div> </div>
1	D	366	<div> <div> <div></div> <div>55%</div> <div>41%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7402 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 Thioredoxin 1,ADP-ribose glycohydrolase MACROD2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	1	0
			1703	1084	299	309	11			
1	B	215	Total	C	N	O	S	0	3	0
			1719	1095	300	312	12			
1	C	218	Total	C	N	O	S	0	3	0
			1743	1111	307	314	11			
1	D	217	Total	C	N	O	S	0	0	0
			1716	1093	299	313	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-122	MET	-	initiating methionine	UNP P0AA25
A	-121	HIS	-	expression tag	UNP P0AA25
A	-120	HIS	-	expression tag	UNP P0AA25
A	-119	HIS	-	expression tag	UNP P0AA25
A	-118	HIS	-	expression tag	UNP P0AA25
A	-117	HIS	-	expression tag	UNP P0AA25
A	-116	HIS	-	expression tag	UNP P0AA25
A	-115	SER	-	expression tag	UNP P0AA25
A	-114	SER	-	expression tag	UNP P0AA25
A	-113	GLY	-	expression tag	UNP P0AA25
A	-3	GLY	-	linker	UNP P0AA25
A	-2	THR	-	linker	UNP P0AA25
A	-1	GLU	-	linker	UNP P0AA25
A	0	ASN	-	linker	UNP P0AA25
A	1	LEU	-	linker	UNP P0AA25
A	2	TYR	-	linker	UNP P0AA25
A	3	PHE	-	linker	UNP P0AA25
A	4	GLN	-	linker	UNP P0AA25
A	5	SER	-	linker	UNP P0AA25
A	6	MET	-	linker	UNP P0AA25
B	-122	MET	-	initiating methionine	UNP P0AA25

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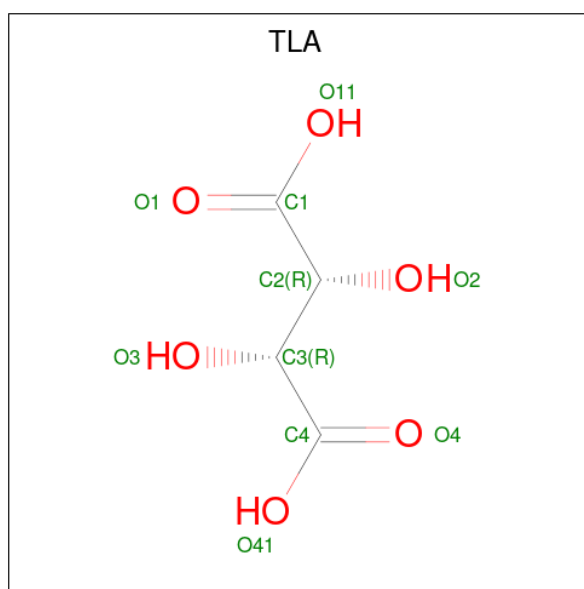
Chain	Residue	Modelled	Actual	Comment	Reference
B	-121	HIS	-	expression tag	UNP P0AA25
B	-120	HIS	-	expression tag	UNP P0AA25
B	-119	HIS	-	expression tag	UNP P0AA25
B	-118	HIS	-	expression tag	UNP P0AA25
B	-117	HIS	-	expression tag	UNP P0AA25
B	-116	HIS	-	expression tag	UNP P0AA25
B	-115	SER	-	expression tag	UNP P0AA25
B	-114	SER	-	expression tag	UNP P0AA25
B	-113	GLY	-	expression tag	UNP P0AA25
B	-3	GLY	-	linker	UNP P0AA25
B	-2	THR	-	linker	UNP P0AA25
B	-1	GLU	-	linker	UNP P0AA25
B	0	ASN	-	linker	UNP P0AA25
B	1	LEU	-	linker	UNP P0AA25
B	2	TYR	-	linker	UNP P0AA25
B	3	PHE	-	linker	UNP P0AA25
B	4	GLN	-	linker	UNP P0AA25
B	5	SER	-	linker	UNP P0AA25
B	6	MET	-	linker	UNP P0AA25
C	-122	MET	-	initiating methionine	UNP P0AA25
C	-121	HIS	-	expression tag	UNP P0AA25
C	-120	HIS	-	expression tag	UNP P0AA25
C	-119	HIS	-	expression tag	UNP P0AA25
C	-118	HIS	-	expression tag	UNP P0AA25
C	-117	HIS	-	expression tag	UNP P0AA25
C	-116	HIS	-	expression tag	UNP P0AA25
C	-115	SER	-	expression tag	UNP P0AA25
C	-114	SER	-	expression tag	UNP P0AA25
C	-113	GLY	-	expression tag	UNP P0AA25
C	-3	GLY	-	linker	UNP P0AA25
C	-2	THR	-	linker	UNP P0AA25
C	-1	GLU	-	linker	UNP P0AA25
C	0	ASN	-	linker	UNP P0AA25
C	1	LEU	-	linker	UNP P0AA25
C	2	TYR	-	linker	UNP P0AA25
C	3	PHE	-	linker	UNP P0AA25
C	4	GLN	-	linker	UNP P0AA25
C	5	SER	-	linker	UNP P0AA25
C	6	MET	-	linker	UNP P0AA25
D	-122	MET	-	initiating methionine	UNP P0AA25
D	-121	HIS	-	expression tag	UNP P0AA25
D	-120	HIS	-	expression tag	UNP P0AA25

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-119	HIS	-	expression tag	UNP P0AA25
D	-118	HIS	-	expression tag	UNP P0AA25
D	-117	HIS	-	expression tag	UNP P0AA25
D	-116	HIS	-	expression tag	UNP P0AA25
D	-115	SER	-	expression tag	UNP P0AA25
D	-114	SER	-	expression tag	UNP P0AA25
D	-113	GLY	-	expression tag	UNP P0AA25
D	-3	GLY	-	linker	UNP P0AA25
D	-2	THR	-	linker	UNP P0AA25
D	-1	GLU	-	linker	UNP P0AA25
D	0	ASN	-	linker	UNP P0AA25
D	1	LEU	-	linker	UNP P0AA25
D	2	TYR	-	linker	UNP P0AA25
D	3	PHE	-	linker	UNP P0AA25
D	4	GLN	-	linker	UNP P0AA25
D	5	SER	-	linker	UNP P0AA25
D	6	MET	-	linker	UNP P0AA25

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			10	4	6		

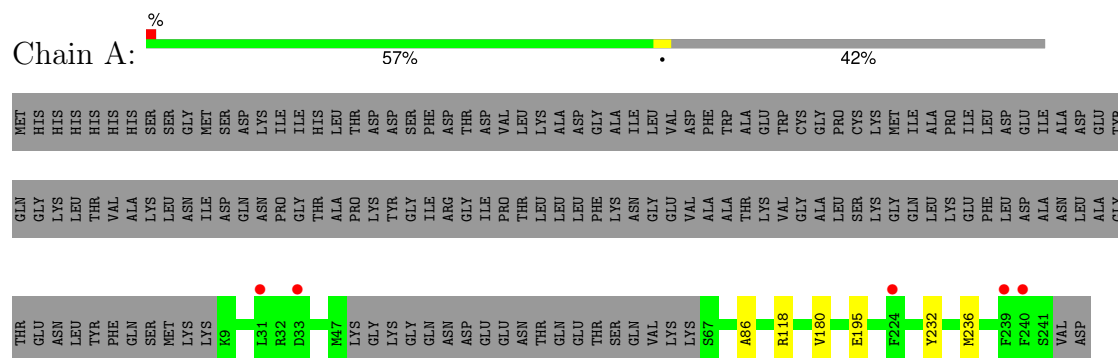
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	138	Total 138	O 138	0	0
3	B	135	Total 135	O 135	0	0
3	C	98	Total 98	O 98	0	0
3	D	140	Total 140	O 140	0	0

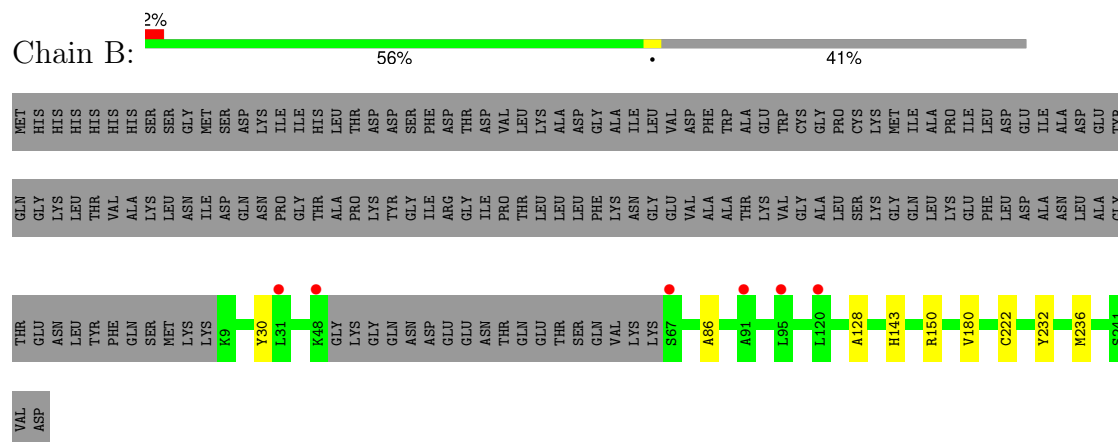
3 Residue-property plots [i](#)

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.

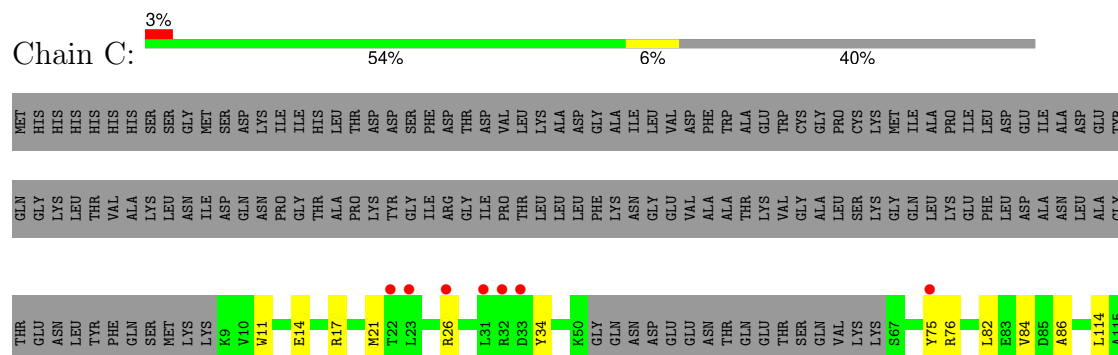
- Molecule 1: Thioredoxin 1,ADP-ribose glycohydrolase MACROD2

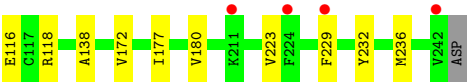


- Molecule 1: Thioredoxin 1,ADP-ribose glycohydrolase MACROD2



- Molecule 1: Thioredoxin 1,ADP-ribose glycohydrolase MACROD2





● Molecule 1: Thioredoxin 1,ADP-ribose glycohydrolase MACROD2



MET	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	ASP	ASP	LYS	ILE	HIS	LEU	THR	ASP	ASP	PHE	THR	ASP	VAL	LEU	LYS	ALA	ASP	GLY	ALA	ILE	LEU	VAL	ASP	PHE	TRP	ALA	GLU	TRP	CYS	GLY	PRO	CYS	LYS	MET	ILE	ALA	PRO	ILE	LEU	ASP	GLU	ILE	ALA	ASP	GLU	TYR
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GLN	GLY	LYS	LEU	THR	VAL	ALA	LYS	LEU	ILE	ASN	GLN	ASN	PRO	GLY	THR	ALA	PRO	LYS	TYR	GLY	ILE	ARG	GLY	ILE	PRO	THR	LEU	LEU	LEU	LEU	PHE	LYS	ASN	GLN	GLY	THR	GLU	VAL	ALA	ALA	THR	LYS	VAL	GLY	ALA	LEU	SER	LYS	GLY	GLN	LEU	LYS	PHE	LEU	ASP	ALA	ASN	LEU	ALA	GLY
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THR	GLU	ASN	LEU	TYR	PHE	GLN	SER	MET	LYS	LYS	K9	R26	E29	Y30	L31	I40	M47	K48	GLY	LYS	GLY	GLN	ASN	ASP	GLU	GLU	ASN	THR	GLN	THR	GLU	THR	SER	GLN	VAL	LYS	S67	R76	L82	E83	V84	L120	C132	G133	Y134	A138	V145	R150
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E195	P196	V223	F224	F229	V242	D243
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4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.65Å 95.65Å 258.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.83 – 1.75 47.83 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.83-1.75) 100.0 (47.83-1.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.204 , 0.227 0.211 , 0.233	Depositor DCC
R_{free} test set	6079 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7402	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TLA

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	0.64	0/1736	0.77	0/2340
1	B	0.67	0/1755	0.79	1/2364 (0.0%)
1	C	0.66	0/1782	0.77	0/2399
1	D	0.66	0/1749	0.77	0/2358
All	All	0.66	0/7022	0.77	1/9461 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	TYR	CB-CG-CD1	6.21	124.73	121.00

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	1703	0	1721	5	0
1	B	1719	0	1743	4	0
1	C	1743	0	1778	13	0
1	D	1716	0	1735	9	0
2	B	10	0	4	0	0
3	A	138	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	135	0	0	0	0
3	C	98	0	0	0	0
3	D	140	0	0	1	0
All	All	7402	0	6981	29	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 2.

The worst 5 of 29 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:223:VAL:HG21	1:C:229:PHE:HB2	1.82	0.62
1:A:232:TYR:O	1:A:236:MET:HG2	2.08	0.54
1:C:21:MET:HE3	1:C:26:ARG:HA	1.89	0.53
1:A:118[B]:ARG:O	1:D:150:ARG:HD3	2.09	0.52
1:D:76:ARG:HD2	1:D:229:PHE:CD1	2.44	0.52

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	211/366 (58%)	210 (100%)	1 (0%)	0	100	100
1	B	214/366 (58%)	211 (99%)	3 (1%)	0	100	100
1	C	217/366 (59%)	215 (99%)	2 (1%)	0	100	100
1	D	213/366 (58%)	210 (99%)	3 (1%)	0	100	100
All	All	855/1464 (58%)	846 (99%)	9 (1%)	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	184/310 (59%)	184 (100%)	0	100	100
1	B	187/310 (60%)	185 (99%)	2 (1%)	73	60
1	C	189/310 (61%)	189 (100%)	0	100	100
1	D	186/310 (60%)	184 (99%)	2 (1%)	73	60
All	All	746/1240 (60%)	742 (100%)	4 (0%)	91	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	222[A]	CYS
1	B	222[B]	CYS
1	D	29	GLU
1	D	47	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

1 ligand is 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	TLA	B	301	-	9,9,9	1.19	0	12,12,12	1.16	2 (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
2	TLA	B	301	-	-	0/12/12/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	TLA	O11-C1-C2	2.21	119.44	113.31
2	B	301	TLA	O41-C4-C3	2.11	119.17	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	214/366 (58%)	0.05	5 (2%) 60 67	22, 32, 58, 73	0
1	B	215/366 (58%)	0.15	6 (2%) 53 58	21, 30, 53, 76	0
1	C	218/366 (59%)	0.16	11 (5%) 28 34	24, 36, 66, 89	0
1	D	217/366 (59%)	0.20	7 (3%) 47 54	20, 30, 56, 85	0
All	All	864/1464 (59%)	0.14	29 (3%) 45 51	20, 32, 59, 89	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	242	VAL	8.9
1	C	31	LEU	4.3
1	B	31	LEU	4.3
1	A	31	LEU	3.9
1	D	224	PHE	3.7

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(\AA^2)	Q<0.9
2	TLA	B	301	10/10	0.95	0.08	27,30,31,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.