



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 15, 2023 – 12:26 AM EDT

PDB ID : 1RII
Title : Crystal structure of phosphoglycerate mutase from M. Tuberculosis
Authors : Mueller, P.; Sawaya, M.R.; Chan, S.; Wu, Y.; Pashkova, I.; Perry, J.; Eisenberg, D.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2003-11-17
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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

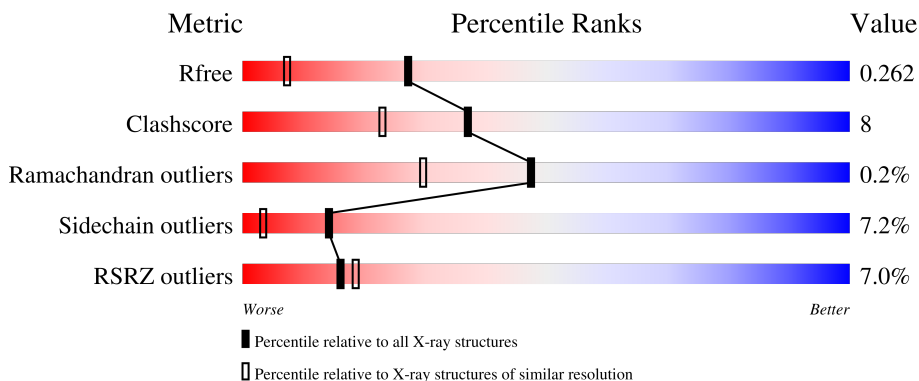
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	265	 5% 74% 15% 8%
1	B	265	 6% 74% 13% 11%
1	C	265	 8% 69% 17% 11%
1	D	265	 6% 73% 12% 13%

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	A	501	-	-	X	-
2	GOL	B	502	-	-	X	-
2	GOL	D	503	-	X	X	-

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7910 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 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1884	1188	338	354	4	0	2	0
1	B	237	1854	1168	334	348	4	0	1	0
1	C	237	1853	1168	331	350	4	0	3	0
1	D	231	1838	1159	331	344	4	0	5	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	GLY	-	cloning artifact	UNP P0A5R6
A	251	VAL	-	cloning artifact	UNP P0A5R6
A	252	PRO	-	cloning artifact	UNP P0A5R6
A	253	ARG	-	cloning artifact	UNP P0A5R6
A	254	GLY	-	cloning artifact	UNP P0A5R6
A	255	ALA	-	cloning artifact	UNP P0A5R6
A	256	ALA	-	cloning artifact	UNP P0A5R6
A	257	ALA	-	cloning artifact	UNP P0A5R6
A	258	LEU	-	cloning artifact	UNP P0A5R6
A	259	GLU	-	cloning artifact	UNP P0A5R6
A	260	HIS	-	cloning artifact	UNP P0A5R6
A	261	HIS	-	cloning artifact	UNP P0A5R6
A	262	HIS	-	cloning artifact	UNP P0A5R6
A	263	HIS	-	cloning artifact	UNP P0A5R6
A	264	HIS	-	cloning artifact	UNP P0A5R6
A	265	HIS	-	cloning artifact	UNP P0A5R6
B	250	GLY	-	cloning artifact	UNP P0A5R6
B	251	VAL	-	cloning artifact	UNP P0A5R6
B	252	PRO	-	cloning artifact	UNP P0A5R6
B	253	ARG	-	cloning artifact	UNP P0A5R6
B	254	GLY	-	cloning artifact	UNP P0A5R6

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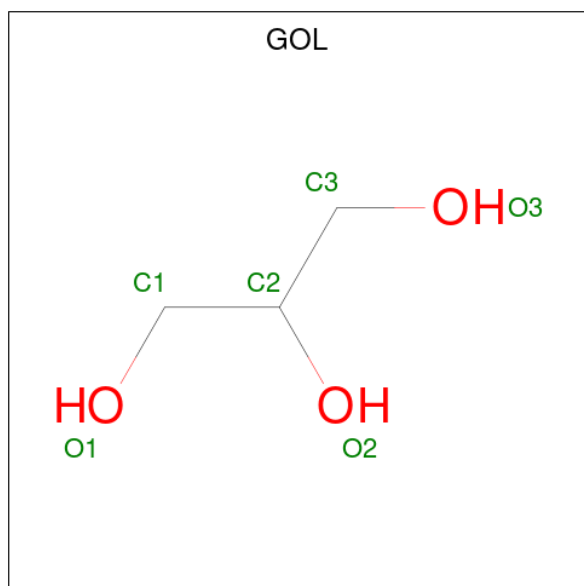
Chain	Residue	Modelled	Actual	Comment	Reference
B	255	ALA	-	cloning artifact	UNP P0A5R6
B	256	ALA	-	cloning artifact	UNP P0A5R6
B	257	ALA	-	cloning artifact	UNP P0A5R6
B	258	LEU	-	cloning artifact	UNP P0A5R6
B	259	GLU	-	cloning artifact	UNP P0A5R6
B	260	HIS	-	cloning artifact	UNP P0A5R6
B	261	HIS	-	cloning artifact	UNP P0A5R6
B	262	HIS	-	cloning artifact	UNP P0A5R6
B	263	HIS	-	cloning artifact	UNP P0A5R6
B	264	HIS	-	cloning artifact	UNP P0A5R6
B	265	HIS	-	cloning artifact	UNP P0A5R6
C	250	GLY	-	cloning artifact	UNP P0A5R6
C	251	VAL	-	cloning artifact	UNP P0A5R6
C	252	PRO	-	cloning artifact	UNP P0A5R6
C	253	ARG	-	cloning artifact	UNP P0A5R6
C	254	GLY	-	cloning artifact	UNP P0A5R6
C	255	ALA	-	cloning artifact	UNP P0A5R6
C	256	ALA	-	cloning artifact	UNP P0A5R6
C	257	ALA	-	cloning artifact	UNP P0A5R6
C	258	LEU	-	cloning artifact	UNP P0A5R6
C	259	GLU	-	cloning artifact	UNP P0A5R6
C	260	HIS	-	cloning artifact	UNP P0A5R6
C	261	HIS	-	cloning artifact	UNP P0A5R6
C	262	HIS	-	cloning artifact	UNP P0A5R6
C	263	HIS	-	cloning artifact	UNP P0A5R6
C	264	HIS	-	cloning artifact	UNP P0A5R6
C	265	HIS	-	cloning artifact	UNP P0A5R6
D	250	GLY	-	cloning artifact	UNP P0A5R6
D	251	VAL	-	cloning artifact	UNP P0A5R6
D	252	PRO	-	cloning artifact	UNP P0A5R6
D	253	ARG	-	cloning artifact	UNP P0A5R6
D	254	GLY	-	cloning artifact	UNP P0A5R6
D	255	ALA	-	cloning artifact	UNP P0A5R6
D	256	ALA	-	cloning artifact	UNP P0A5R6
D	257	ALA	-	cloning artifact	UNP P0A5R6
D	258	LEU	-	cloning artifact	UNP P0A5R6
D	259	GLU	-	cloning artifact	UNP P0A5R6
D	260	HIS	-	cloning artifact	UNP P0A5R6
D	261	HIS	-	cloning artifact	UNP P0A5R6
D	262	HIS	-	cloning artifact	UNP P0A5R6
D	263	HIS	-	cloning artifact	UNP P0A5R6
D	264	HIS	-	cloning artifact	UNP P0A5R6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	265	HIS	-	cloning artifact	UNP P0A5R6

- Molecule 2 is GLYCEROL (three-letter code: 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	D	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

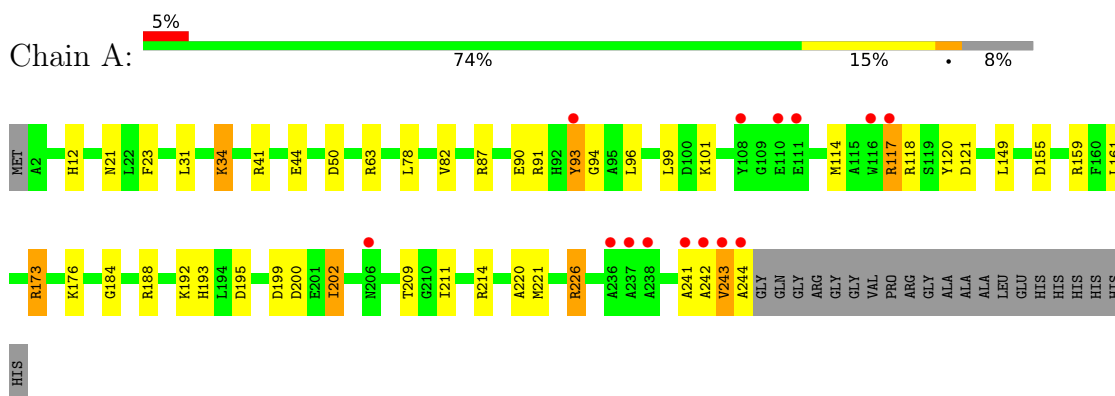
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	112	Total O 112 112	0	0
3	B	134	Total O 134 134	0	0
3	C	87	Total O 87 87	0	0
3	D	118	Total O 118 118	0	0

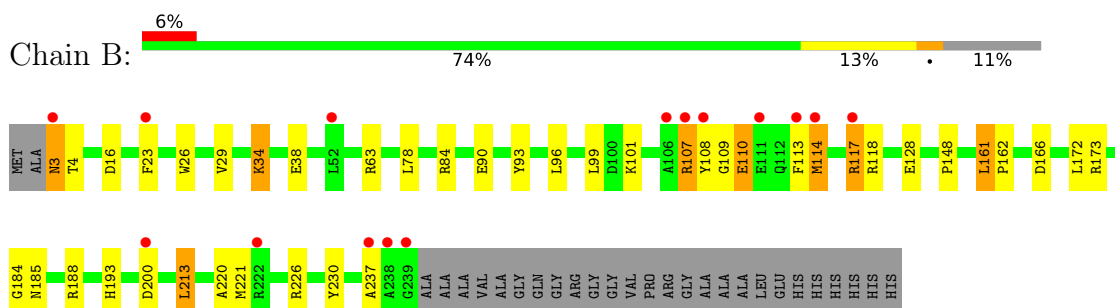
3 Residue-property plots [i](#)

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.

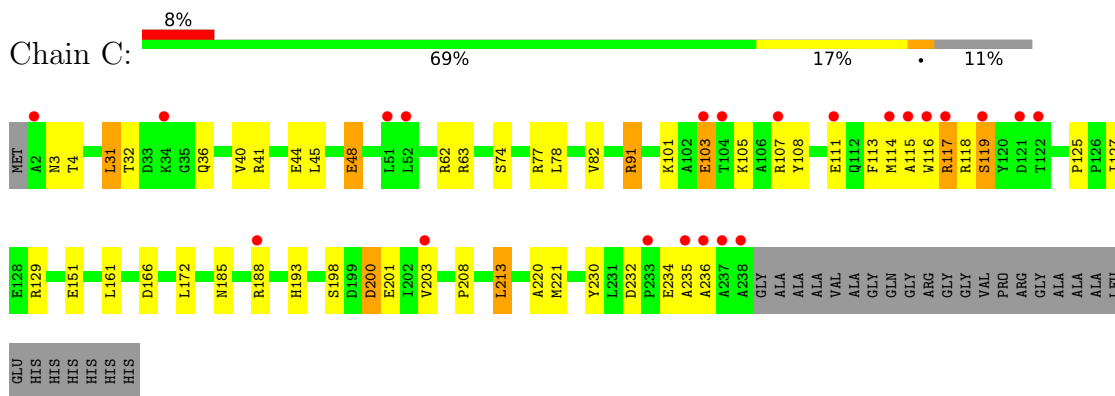
- Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase



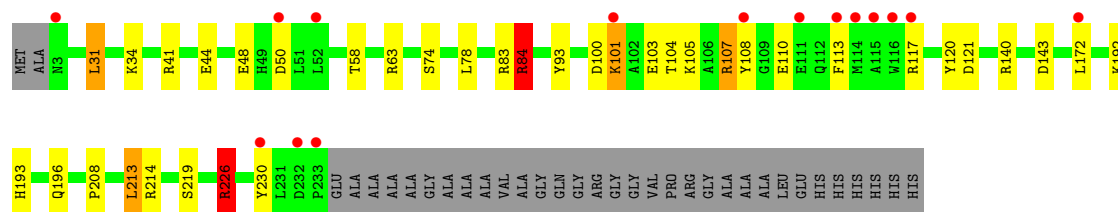
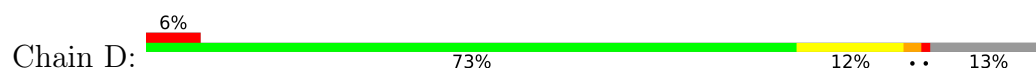
- Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase



- Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase



- Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.91Å 136.79Å 65.93Å 90.00° 97.78° 90.00°	Depositor
Resolution (Å)	58.37 – 1.70 58.37 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (58.37-1.70) 94.4 (58.37-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.70Å)	Xtrriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.221 , 0.270 0.216 , 0.262	Depositor DCC
R_{free} test set	2677 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtrriage
Anisotropy	0.261	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7910	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: 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	0.34	0/1933	0.97	2/2634 (0.1%)
1	B	0.35	0/1899	1.01	3/2585 (0.1%)
1	C	0.33	0/1906	1.01	4/2597 (0.2%)
1	D	0.35	0/1899	1.06	7/2584 (0.3%)
All	All	0.35	0/7637	1.01	16/10400 (0.2%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	D	226	ARG	CD-NE-CZ	7.78	134.49	123.60
1	D	84[A]	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	D	84[B]	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	84	ARG	NE-CZ-NH2	-7.47	116.57	120.30

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	1884	0	1859	32	0
1	B	1854	0	1829	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1853	0	1816	27	0
1	D	1838	0	1809	29	0
2	A	6	0	8	4	0
2	B	6	0	7	5	0
2	D	18	0	22	5	0
3	A	112	0	0	2	0
3	B	134	0	0	0	0
3	C	87	0	0	2	0
3	D	118	0	0	2	0
All	All	7910	0	7350	116	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 8.

The worst 5 of 116 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:D:83[A]:ARG:HE	2:D:505:GOL:H32	1.40	0.85
1:D:63:ARG:HE	2:D:503:GOL:H32	1.42	0.83
1:A:93:TYR:OH	1:A:117:ARG:HG3	1.85	0.75
1:B:63:ARG:NE	2:B:502:GOL:H12	2.03	0.74
1:B:110:GLU:OE2	1:B:114:MET:HG2	1.87	0.74

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	243/265 (92%)	234 (96%)	8 (3%)	1 (0%)	34 18
1	B	236/265 (89%)	232 (98%)	3 (1%)	1 (0%)	34 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	238/265 (90%)	234 (98%)	4 (2%)	0	100	100
1	D	234/265 (88%)	229 (98%)	5 (2%)	0	100	100
All	All	951/1060 (90%)	929 (98%)	20 (2%)	2 (0%)	47	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	VAL
1	B	237	ALA

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	195/208 (94%)	182 (93%)	13 (7%)	16	4
1	B	194/208 (93%)	178 (92%)	16 (8%)	11	2
1	C	194/208 (93%)	180 (93%)	14 (7%)	14	3
1	D	196/208 (94%)	179 (91%)	17 (9%)	10	2
All	All	779/832 (94%)	719 (92%)	60 (8%)	14	3

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	226[B]	ARG
1	D	213	LEU
1	C	111	GLU
1	D	172	LEU
1	D	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	132	GLN
1	C	3	ASN
1	C	112	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	505	-	5,5,5	0.82	0	5,5,5	1.55	1 (20%)
2	GOL	D	503	-	5,5,5	0.96	0	5,5,5	1.72	2 (40%)
2	GOL	B	502	-	5,5,5	0.89	0	5,5,5	2.07	3 (60%)
2	GOL	A	501	-	5,5,5	0.88	0	5,5,5	1.71	2 (40%)
2	GOL	D	504	-	5,5,5	0.68	0	5,5,5	1.11	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	505	-	-	2/4/4/4	-
2	GOL	D	503	-	-	4/4/4/4	-
2	GOL	B	502	-	-	2/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-
2	GOL	D	504	-	-	2/4/4/4	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	GOL	O1-C1-C2	3.23	125.68	110.20
2	A	501	GOL	O3-C3-C2	3.11	125.10	110.20
2	D	503	GOL	O3-C3-C2	3.00	124.60	110.20
2	D	505	GOL	O1-C1-C2	2.62	122.78	110.20
2	D	503	GOL	O1-C1-C2	2.38	121.61	110.20

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	C1-C2-C3-O3
2	A	501	GOL	O2-C2-C3-O3
2	D	503	GOL	C1-C2-C3-O3
2	D	503	GOL	O2-C2-C3-O3
2	D	504	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	505	GOL	1	0
2	D	503	GOL	4	0
2	B	502	GOL	5	0
2	A	501	GOL	4	0

5.7 Other polymers [\(i\)](#)

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	243/265 (91%)	0.71	14 (5%) 23 25	21, 30, 53, 91	0
1	B	237/265 (89%)	0.73	15 (6%) 20 22	21, 29, 52, 71	0
1	C	237/265 (89%)	0.82	22 (9%) 8 9	24, 34, 57, 80	0
1	D	231/265 (87%)	0.61	15 (6%) 18 21	21, 30, 54, 68	0
All	All	948/1060 (89%)	0.72	66 (6%) 16 18	21, 30, 55, 91	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	10.8
1	A	243	VAL	9.8
1	B	238	ALA	9.4
1	A	244	ALA	8.6
1	A	242	ALA	7.4

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	GOL	D	505	6/6	0.59	0.30	49,53,54,57	0
2	GOL	D	504	6/6	0.67	0.15	45,48,50,53	0
2	GOL	B	502	6/6	0.86	0.19	31,38,41,42	0
2	GOL	A	501	6/6	0.87	0.29	32,44,46,46	0
2	GOL	D	503	6/6	0.92	0.28	15,23,24,29	6

6.5 Other polymers [i](#)

There are no such residues in this entry.