



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 01:51 AM EDT

PDB ID : 7JH0
Title : Crystallographic structure of glyceraldehyde-3-phosphate dehydrogenase from Schistosoma mansoni
Authors : Boreiko, S.; Silva, M.; Iulek, J.
Deposited on : 2020-07-20
Resolution : 2.51 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 : 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

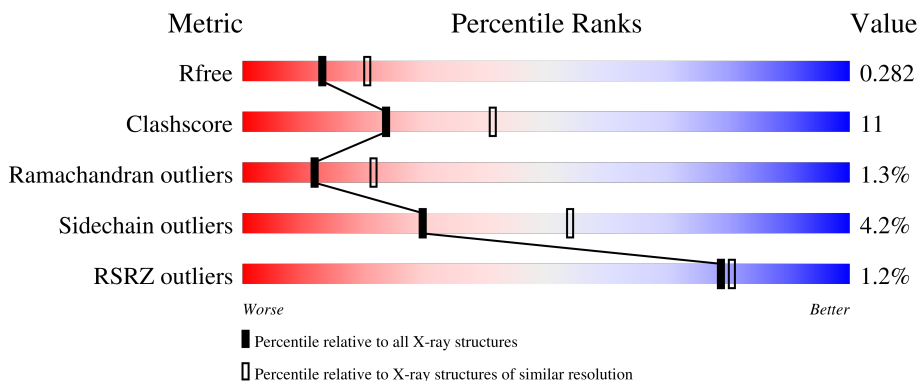
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



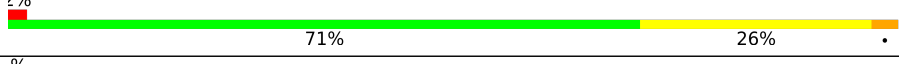

The reported resolution of this entry is 2.51 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	338	 75% 23%
1	B	338	 2% 76% 22%
1	C	338	 2% 71% 26%
2	D	338	 2% 73% 25%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10188 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.

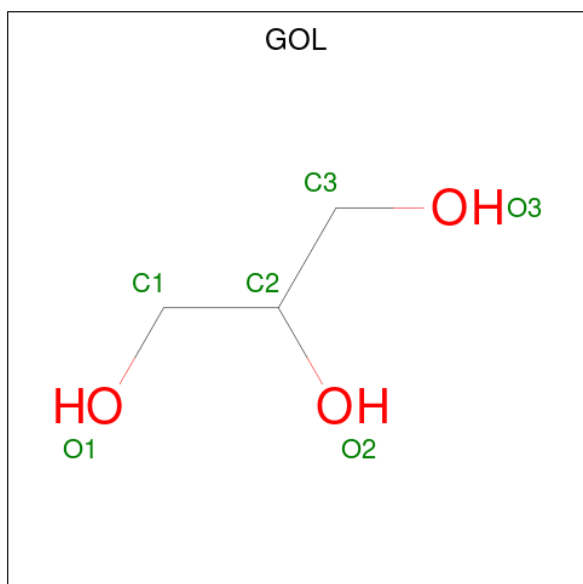
- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	338	Total 2512	C 1580	N 429	O 488	P 1	S 14	0	2	0
1	B	338	Total 2476	C 1549	N 431	O 482	P 1	S 13	0	3	0
1	C	338	Total 2481	C 1559	N 429	O 478	P 1	S 14	0	1	0

- Molecule 2 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

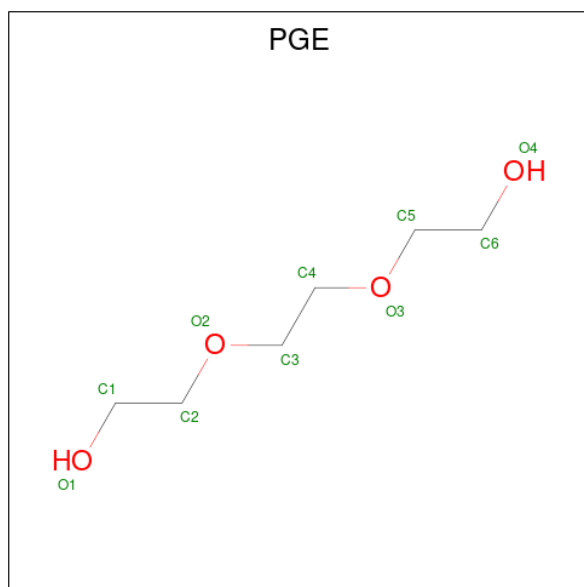
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	338	Total 2466	C 1551	N 426	O 476	S 13	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

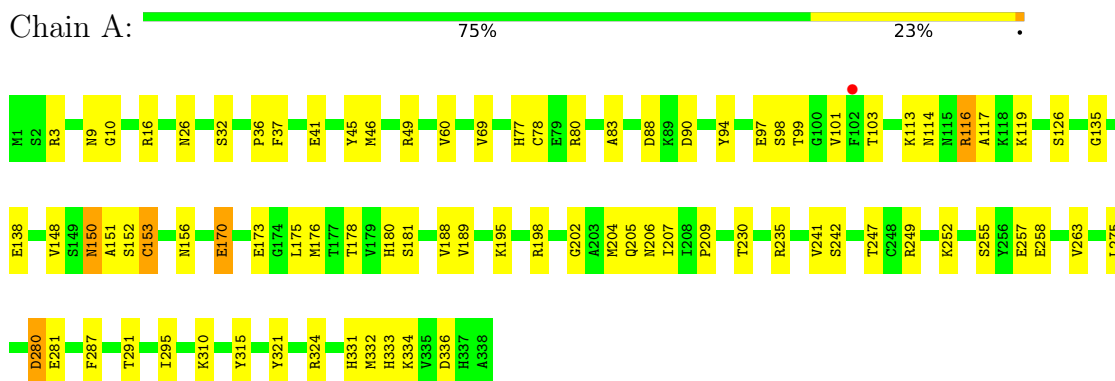
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	45	Total O 45 45	0	0
7	B	57	Total O 57 57	0	0
7	C	49	Total O 49 49	0	0
7	D	52	Total O 52 52	0	0

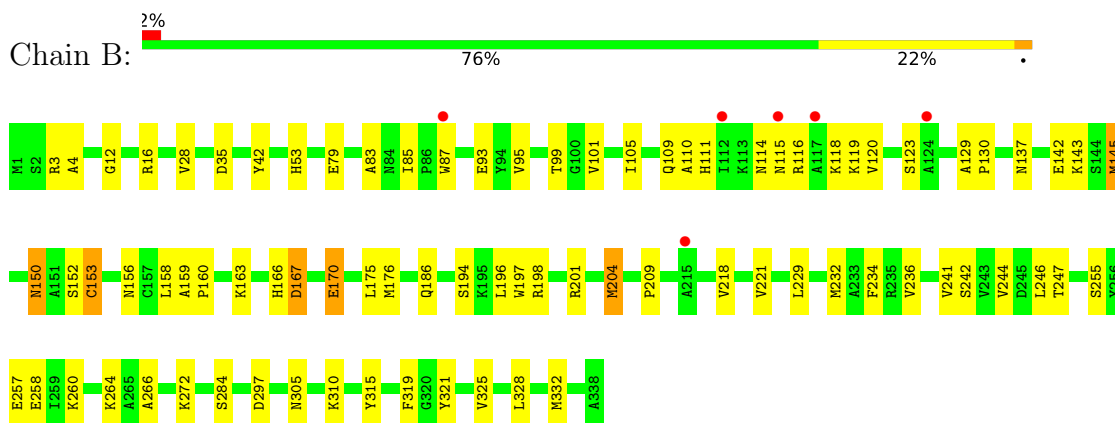
3 Residue-property plots

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.

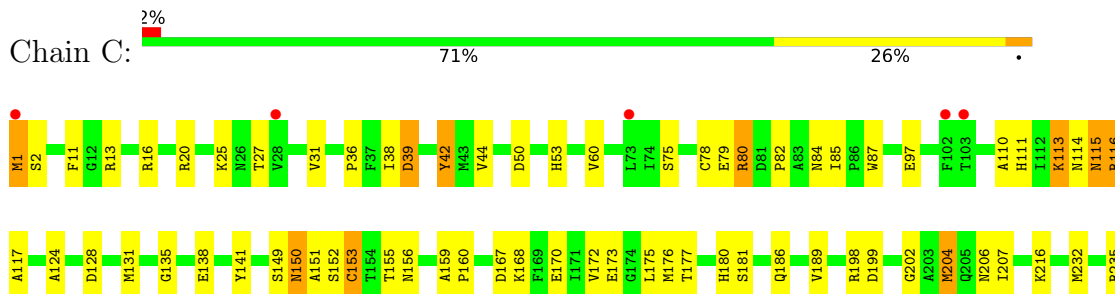
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

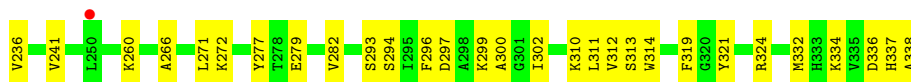


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

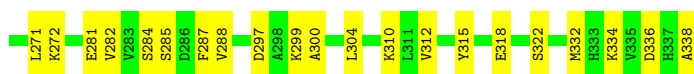
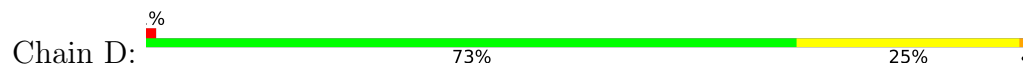


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase





● Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	80.12Å 80.12Å 417.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.76 – 2.51 57.76 – 2.51	Depositor EDS
% Data completeness (in resolution range)	100.0 (57.76-2.51) 100.0 (57.76-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.213 , 0.273 0.222 , 0.282	Depositor DCC
R_{free} test set	1967 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtrriage
Anisotropy	0.350	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.087 for h,-h-k,-l	Xtrriage
Reported twinning fraction	0.080 for h,-h-k,-l	Depositor
Outliers	1 of 51375 reflections (0.002%)	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10188	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: EDO, PEG, CSD, CSP, PGE, 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	0.26	0/2560	0.42	0/3473
1	B	0.26	0/2526	0.42	0/3433
1	C	0.28	0/2521	0.44	0/3422
2	D	0.27	0/2504	0.43	0/3407
All	All	0.27	0/10111	0.43	0/13735

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	2512	0	2430	62	0
1	B	2476	0	2353	58	0
1	C	2481	0	2378	62	0
2	D	2466	0	2353	61	0
3	A	6	0	8	1	0
3	B	6	0	8	1	0
4	A	10	0	14	2	0
4	B	10	0	14	2	0
5	B	7	0	10	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	7	0	10	3	0
6	C	4	0	6	1	0
7	A	45	0	0	4	0
7	B	57	0	0	7	0
7	C	49	0	0	0	0
7	D	52	0	0	0	0
All	All	10188	0	9584	219	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 219 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:114:ASN:O	1:C:115:ASN:ND2	2.01	0.92
1:C:332:MET:O	1:C:336:ASP:N	2.06	0.88
2:D:110:ALA:O	2:D:116:ARG:NH1	2.07	0.88
1:A:49:ARG:HH12	1:C:282:VAL:HG12	1.42	0.85
1:A:249:ARG:HD2	2:D:249:ARG:HD2	1.61	0.82

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	337/338 (100%)	316 (94%)	19 (6%)	2 (1%)	25 43
1	B	338/338 (100%)	306 (90%)	27 (8%)	5 (2%)	10 18
1	C	336/338 (99%)	298 (89%)	33 (10%)	5 (2%)	10 18
2	D	335/338 (99%)	299 (89%)	30 (9%)	6 (2%)	8 14
All	All	1346/1352 (100%)	1219 (91%)	109 (8%)	18 (1%)	12 21

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	ASN
1	A	170	GLU
1	B	170	GLU
1	B	241	VAL
1	C	241	VAL

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	261/280 (93%)	251 (96%)	10 (4%)	33 58
1	B	249/280 (89%)	241 (97%)	8 (3%)	39 65
1	C	250/280 (89%)	232 (93%)	18 (7%)	14 28
2	D	247/280 (88%)	241 (98%)	6 (2%)	49 74
All	All	1007/1120 (90%)	965 (96%)	42 (4%)	30 54

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	150	ASN
1	C	334	LYS
1	C	168	LYS
1	C	216	LYS
2	D	42	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	337	HIS
2	D	53	HIS
2	D	337	HIS
2	D	139	ASN
1	B	205	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](#)

4 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	CSP	A	153	1	6,9,10	2.05	1 (16%)	3,12,14	2.65	1 (33%)
1	CSP	B	153	1	6,9,10	2.06	1 (16%)	3,12,14	4.51	3 (100%)
2	CSD	D	153	2	3,7,8	1.20	0	1,8,10	1.69	0
1	CSP	C	153	1	6,9,10	2.02	1 (16%)	3,12,14	4.85	3 (100%)

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	CSP	A	153	1	-	0/0/8/10	-
1	CSP	B	153	1	-	0/0/8/10	-
2	CSD	D	153	2	-	1/2/6/8	-
1	CSP	C	153	1	-	0/0/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	CSP	P-O3P	-4.70	1.44	1.56
1	B	153	CSP	P-O2P	-4.69	1.44	1.56
1	C	153	CSP	P-O3P	-4.62	1.44	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	153	CSP	O2P-P-O1P	-7.35	95.95	112.98
1	B	153	CSP	O3P-P-O1P	-6.38	98.20	112.98
1	A	153	CSP	O2P-P-O1P	-4.58	102.36	112.98
1	B	153	CSP	CA-CB-SG	-3.58	105.32	112.76
1	C	153	CSP	CA-CB-SG	-3.42	105.64	112.76

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	153	CSD	CA-CB-SG-OD1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	153	CSP	1	0
1	B	153	CSP	1	0
1	C	153	CSP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
5	PEG	B	402	-	6,6,6	0.09	0	5,5,5	0.16	0
3	GOL	A	401	-	5,5,5	0.08	0	5,5,5	0.22	0
5	PEG	D	401	-	6,6,6	0.14	0	5,5,5	0.07	0
4	PGE	B	403	-	9,9,9	0.16	0	8,8,8	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	C	401	-	3,3,3	0.07	0	2,2,2	0.15	0
3	GOL	B	401	-	5,5,5	0.09	0	5,5,5	0.33	0
4	PGE	A	402	-	9,9,9	0.14	0	8,8,8	0.11	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
5	PEG	B	402	-	-	1/4/4/4	-
3	GOL	A	401	-	-	4/4/4/4	-
5	PEG	D	401	-	-	3/4/4/4	-
4	PGE	B	403	-	-	5/7/7/7	-
6	EDO	C	401	-	-	0/1/1/1	-
3	GOL	B	401	-	-	3/4/4/4	-
4	PGE	A	402	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GOL	O1-C1-C2-O2
3	A	401	GOL	O1-C1-C2-C3
3	A	401	GOL	C1-C2-C3-O3
3	A	401	GOL	O2-C2-C3-O3
4	B	403	PGE	C4-C3-O2-C2

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	402	PEG	1	0
3	A	401	GOL	1	0
5	D	401	PEG	3	0
4	B	403	PGE	2	0
6	C	401	EDO	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	GOL	1	0
4	A	402	PGE	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	337/338 (99%)	-0.03	1 (0%) 94 94	46, 66, 95, 124	0
1	B	337/338 (99%)	0.09	6 (1%) 68 71	46, 73, 98, 141	0
1	C	337/338 (99%)	0.13	6 (1%) 68 71	45, 80, 116, 130	0
2	D	337/338 (99%)	-0.00	3 (0%) 84 86	48, 73, 107, 166	0
All	All	1348/1352 (99%)	0.05	16 (1%) 79 80	45, 73, 104, 166	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	3.3
1	C	250	LEU	2.8
1	C	73	LEU	2.7
1	C	103	THR	2.7
1	B	124	ALA	2.7

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
2	CSD	D	153	8/9	0.80	0.18	63,68,80,83	0
1	CSP	C	153	10/11	0.88	0.15	70,85,103,104	0
1	CSP	A	153	10/11	0.88	0.16	60,71,101,104	0
1	CSP	B	153	10/11	0.91	0.17	78,83,98,99	0

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
4	PGE	A	402	10/10	0.77	0.37	98,106,109,110	0
5	PEG	D	401	7/7	0.79	0.17	63,64,66,66	0
5	PEG	B	402	7/7	0.80	0.31	77,79,84,86	0
4	PGE	B	403	10/10	0.82	0.19	78,80,85,85	0
3	GOL	B	401	6/6	0.85	0.15	69,71,74,75	0
3	GOL	A	401	6/6	0.88	0.30	79,81,84,86	0
6	EDO	C	401	4/4	0.91	0.32	66,67,69,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.