



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 03:58 AM EST

PDB ID : 7U4S  
Title : Structure of Glyceraldehyde-3-Phosphate Dehydrogenase from *Candida albicans*  
Authors : Miranda, R.R.; Silva, M.; Iulek, J.  
Deposited on : 2022-02-28  
Resolution : 2.68 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](mailto: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>.

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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 : 2.36  
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) : 2.36

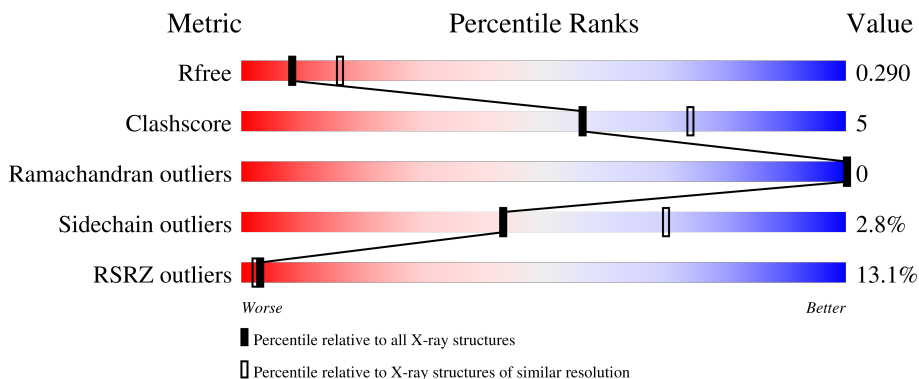
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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  $\geq 3$ , 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	335	
1	B	335	
1	C	335	
1	D	335	

## 2 Entry composition [i](#)

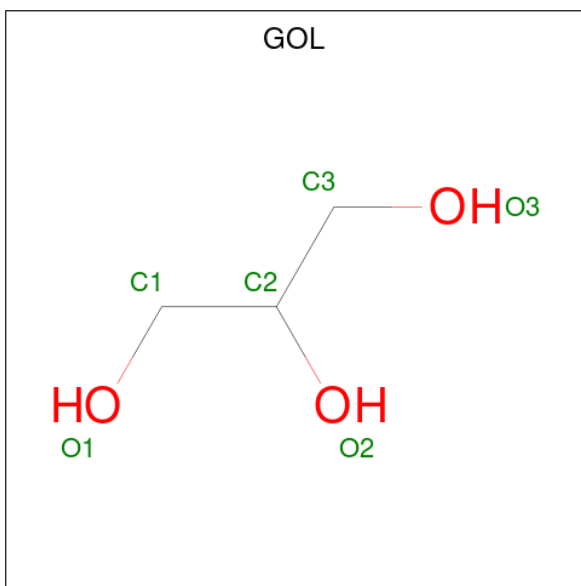
There are 3 unique types of molecules in this entry. The entry contains 10110 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	S			
1	A	327	Total 2450	C 1559	N 403	O 482	S 6	0	8	0
1	B	325	Total 2430	C 1552	N 397	O 473	S 8	0	3	0
1	C	328	Total 2373	C 1512	N 388	O 467	S 6	0	3	0
1	D	325	Total 2377	C 1516	N 388	O 466	S 7	0	2	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

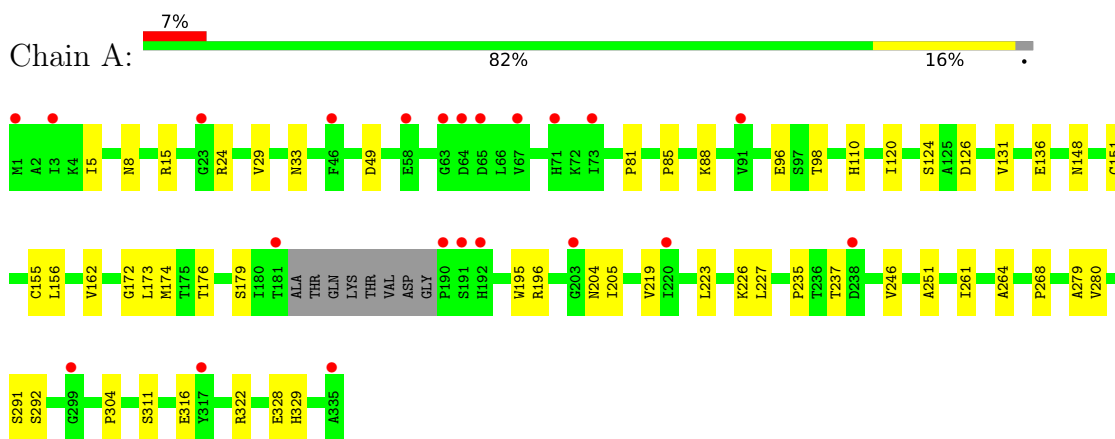
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	128	128	128	0	0
3	B	164	164	164	0	0
3	C	86	86	86	0	0
3	D	84	84	84	0	0

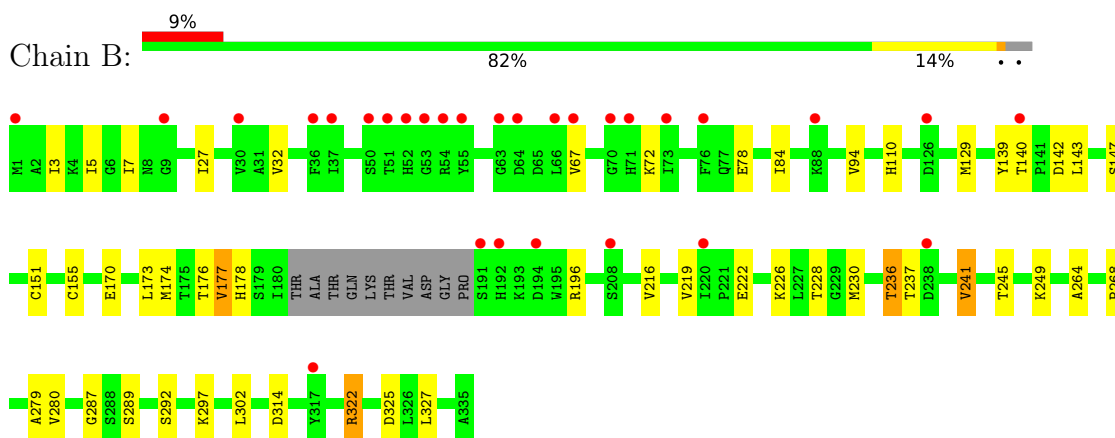
### 3 Residue-property plots [i](#)

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.

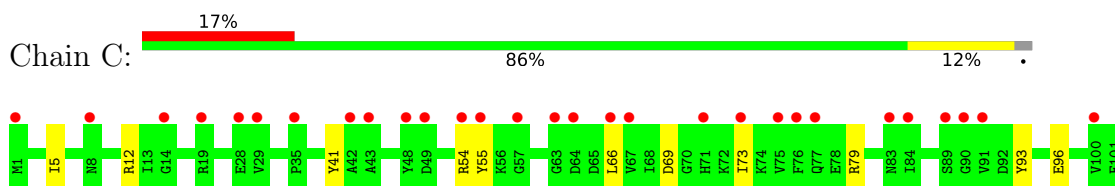
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

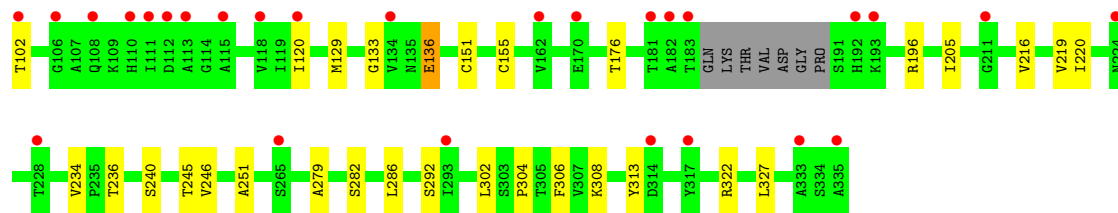


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

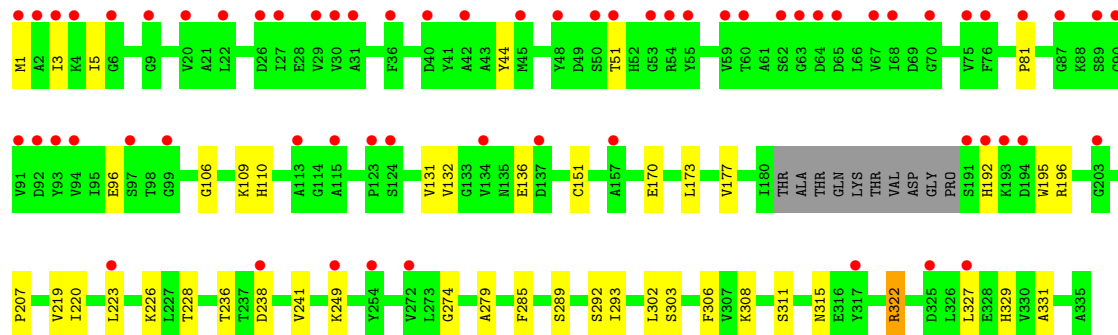
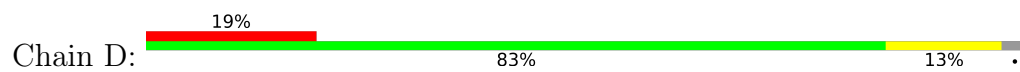


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase





● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.72Å 126.90Å 86.82Å 90.00° 100.32° 90.00°	Depositor
Resolution (Å)	72.52 – 2.68 85.41 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (72.52-2.68) 91.7 (85.41-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.236 , 0.286 0.242 , 0.290	Depositor DCC
$R_{free}$ test set	2192 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtrriage
Anisotropy	0.901	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	10110	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OCS, 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	0.24	0/2537	0.46	0/3443
1	B	0.24	0/2479	0.44	0/3363
1	C	0.24	0/2422	0.45	0/3297
1	D	0.24	0/2423	0.45	0/3300
All	All	0.24	0/9861	0.45	0/13403

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	2450	0	2393	33	0
1	B	2430	0	2407	28	0
1	C	2373	0	2270	21	0
1	D	2377	0	2285	30	0
2	B	12	0	16	0	0
2	D	6	0	8	0	0
3	A	128	0	0	0	0
3	B	164	0	0	1	0
3	C	86	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	84	0	0	0	0
All	All	10110	0	9379	95	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 5.

All (95) 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:A:196:ARG:HG3	1:C:279:ALA:HB1	1.70	0.73
1:B:196:ARG:HG3	1:D:279:ALA:HB1	1.71	0.71
1:B:5:ILE:HG21	1:B:327:LEU:HD21	1.74	0.69
1:C:5:ILE:HG21	1:C:327:LEU:HD21	1.75	0.68
1:D:274:GLY:HA3	1:D:293:ILE:HD13	1.76	0.66
1:D:5:ILE:HG21	1:D:327:LEU:HD21	1.78	0.65
1:B:289:SER:O	1:B:322:ARG:NH2	2.30	0.65
1:C:66:LEU:HB3	1:C:73:ILE:HB	1.81	0.63
1:B:155:CYS:HA	1:B:292:SER:HB3	1.82	0.62
1:D:81:PRO:HG2	1:D:109:LYS:HD2	1.82	0.61
1:A:280:VAL:O	1:C:196:ARG:NH1	2.34	0.60
1:B:228:THR:HG22	1:D:302:LEU:HD12	1.83	0.60
1:B:287:GLY:N	1:B:314:ASP:OD2	2.33	0.60
1:D:289:SER:O	1:D:322:ARG:NH2	2.31	0.58
1:D:170:GLU:HG2	1:D:249:LYS:HG2	1.86	0.58
1:A:173:LEU:HD13	1:C:308:LYS:HB2	1.87	0.57
1:C:5:ILE:HG22	1:C:93:TYR:HB2	1.86	0.56
1:C:205[B]:ILE:HD12	1:C:234:VAL:HG12	1.88	0.55
1:A:85:PRO:HB3	1:A:88:LYS:HE2	1.89	0.54
1:A:173:LEU:HD21	1:C:302:LEU:HB2	1.89	0.54
1:B:3:ILE:HD11	1:B:27:ILE:HG12	1.88	0.54
1:B:196:ARG:NH1	3:B:510:HOH:O	2.37	0.53
1:D:292:SER:OG	1:D:311:SER:OG	2.26	0.53
1:D:96:GLU:OE1	1:D:110:HIS:NE2	2.41	0.53
1:A:172:GLY:HA3	1:A:246:VAL:HG12	1.91	0.53
1:A:126:ASP:N	1:A:126:ASP:OD1	2.42	0.52
1:A:8:ASN:OD1	1:A:33:ASN:ND2	2.38	0.52
1:D:177:VAL:HB	1:D:241:VAL:HG12	1.92	0.52
1:B:67:VAL:HG22	1:B:72:LYS:HG2	1.92	0.51
1:D:192:HIS:HB2	1:D:195:TRP:HE1	1.74	0.51
1:A:120:ILE:HD11	1:A:124:SER:HB2	1.92	0.51
1:B:297:LYS:HB2	1:D:196:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:THR:HG22	1:C:120:ILE:HD11	1.94	0.50
1:D:136:GLU:O	1:D:329:HIS:NE2	2.44	0.50
1:B:280:VAL:O	1:D:196:ARG:NH1	2.44	0.50
1:A:279:ALA:HB1	1:C:196:ARG:HG3	1.94	0.49
1:A:173:LEU:HD12	1:C:245:THR:HG23	1.92	0.49
1:C:219:VAL:HG23	1:C:220:ILE:HG13	1.95	0.49
1:D:131:VAL:HG23	1:D:219:VAL:HG11	1.94	0.49
1:A:24[B]:ARG:NH1	1:A:328:GLU:OE2	2.44	0.48
1:B:302:LEU:HD13	1:D:228:THR:HG22	1.95	0.48
1:B:236:THR:HG22	1:B:237:THR:H	1.79	0.48
1:D:285:PHE:CE1	1:D:293:ILE:HG21	2.49	0.48
1:B:129[A]:MET:HG2	1:B:147:SER:HB3	1.97	0.47
1:C:129:MET:HB3	1:C:129:MET:HE2	1.80	0.47
1:D:238:ASP:O	1:D:315:ASN:ND2	2.48	0.47
1:A:179:SER:HB3	1:A:237:THR:HA	1.96	0.47
1:C:216:VAL:HA	1:C:219:VAL:HG22	1.96	0.47
1:B:177:VAL:HG23	1:B:241:VAL:HG13	1.97	0.46
1:A:131:VAL:HG23	1:A:219:VAL:HG11	1.96	0.46
1:D:106:GLY:HA2	1:D:109:LYS:NZ	2.31	0.46
1:B:264:ALA:HA	1:B:268:PRO:HD2	1.98	0.46
1:B:322:ARG:NH1	1:B:325:ASP:OD2	2.48	0.46
1:B:7:ILE:HB	1:B:32:VAL:HG13	1.98	0.46
1:A:292:SER:OG	1:A:311:SER:OG	2.22	0.46
1:B:173:LEU:HD13	1:D:308:LYS:HB2	1.98	0.46
1:A:81:PRO:HB3	1:A:110:HIS:CE1	2.51	0.46
1:A:223:LEU:HD13	1:A:227:LEU:HD11	1.98	0.45
1:B:216:VAL:HA	1:B:219:VAL:HG12	1.98	0.45
1:D:132:VAL:HA	1:D:136:GLU:HB3	1.99	0.45
1:A:204:ASN:H	1:A:235:PRO:HG3	1.82	0.44
1:A:291:SER:OG	1:A:322:ARG:NH1	2.40	0.44
1:A:156:LEU:HD22	1:A:174:MET:SD	2.58	0.44
1:D:3:ILE:HG21	1:D:331:ALA:HB1	1.98	0.44
1:D:223:LEU:HA	1:D:226:LYS:HD2	2.00	0.44
1:A:264:ALA:HA	1:A:268:PRO:HD2	1.99	0.44
1:B:302:LEU:HB2	1:D:173:LEU:HD21	1.98	0.44
1:A:15:ARG:NH1	1:A:49:ASP:O	2.51	0.43
1:A:96:GLU:HB3	1:A:120:ILE:HA	2.00	0.43
1:A:155:CYS:HA	1:A:292:SER:HB2	2.01	0.43
1:C:155:CYS:HA	1:C:292:SER:HB2	1.99	0.43
1:A:148:ASN:O	1:A:148:ASN:ND2	2.52	0.43
1:D:303:SER:HB3	1:D:306:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ARG:HD3	1:D:207:PRO:HG2	2.01	0.42
1:B:222:GLU:O	1:B:226:LYS:HE2	2.19	0.42
1:A:5:ILE:HD11	1:A:29:VAL:HG22	2.00	0.42
1:D:219:VAL:HG23	1:D:220:ILE:HG13	2.02	0.42
1:A:205:ILE:HB	1:C:282:SER:HB3	2.02	0.42
1:A:223:LEU:HA	1:A:226:LYS:HD2	2.01	0.42
1:C:55:TYR:OH	1:C:69:ASP:OD2	2.31	0.42
1:A:96:GLU:OE2	1:A:98:THR:OG1	2.23	0.42
1:A:251:ALA:HB1	1:A:304:PRO:HB2	2.02	0.42
1:B:94:VAL:HG11	1:B:110:HIS:CG	2.54	0.42
1:C:54:ARG:N	3:C:407:HOH:O	2.53	0.41
1:B:140:THR:OG1	1:B:142:ASP:OD1	2.33	0.41
1:C:133:GLY:N	1:C:136:GLU:OE1	2.50	0.41
1:B:279:ALA:HB1	1:D:196:ARG:HG3	2.03	0.41
1:A:195:TRP:HB3	1:D:44:TYR:CE2	2.56	0.41
1:C:251:ALA:HB1	1:C:304:PRO:HB2	2.02	0.41
1:A:162:VAL:HG11	1:A:261:ILE:HA	2.03	0.41
1:A:136:GLU:O	1:A:329:HIS:NE2	2.54	0.41
1:B:78:GLU:HB2	1:B:84:ILE:HG12	2.04	0.40
1:B:245:THR:HG23	1:D:173:LEU:HD12	2.02	0.40
1:C:240:SER:HB2	1:C:313:TYR:CZ	2.56	0.40
1:B:139:TYR:CE1	1:B:143:LEU:HB2	2.56	0.40

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	331/335 (99%)	306 (92%)	25 (8%)	0	100	100
1	B	323/335 (96%)	298 (92%)	25 (8%)	0	100	100
1	C	326/335 (97%)	292 (90%)	34 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	322/335 (96%)	298 (92%)	24 (8%)	0	100	100
All	All	1302/1340 (97%)	1194 (92%)	108 (8%)	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	256/271 (94%)	253 (99%)	3 (1%)	71	87
1	B	251/271 (93%)	241 (96%)	10 (4%)	31	57
1	C	232/271 (86%)	221 (95%)	11 (5%)	26	50
1	D	237/271 (88%)	233 (98%)	4 (2%)	60	82
All	All	976/1084 (90%)	948 (97%)	28 (3%)	43	69

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	THR
1	A	316[A]	GLU
1	A	316[B]	GLU
1	B	170	GLU
1	B	174	MET
1	B	176	THR
1	B	177	VAL
1	B	178	HIS
1	B	230	MET
1	B	236	THR
1	B	241	VAL
1	B	249	LYS
1	B	322	ARG
1	C	12	ARG
1	C	41	TYR
1	C	79	ARG

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Mol	Chain	Res	Type
1	C	96	GLU
1	C	136	GLU
1	C	176	THR
1	C	236	THR
1	C	246	VAL
1	C	286	LEU
1	C	306	PHE
1	C	322	ARG
1	D	1	MET
1	D	51	THR
1	D	236	THR
1	D	322	ARG

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](#)

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	OCS	A	151	1	2,7,9	0.77	0	2,8,13	2.64	2 (100%)
1	OCS	D	151	1	7,8,9	0.94	0	6,11,13	1.75	2 (33%)
1	OCS	C	151	1	7,8,9	0.94	0	6,11,13	1.73	2 (33%)
1	OCS	B	151	1	2,7,9	0.80	0	2,8,13	2.83	2 (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	OCS	A	151	1	-	1/3/6/9	-
1	OCS	D	151	1	-	0/4/7/9	-
1	OCS	C	151	1	-	0/4/7/9	-
1	OCS	B	151	1	-	1/3/6/9	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	OCS	OD1-SG-CB	2.87	109.51	105.35
1	B	151	OCS	OD3-SG-CB	2.80	109.41	105.35
1	A	151	OCS	OD1-SG-CB	2.65	109.20	105.35
1	A	151	OCS	OD3-SG-CB	2.63	109.17	105.35
1	D	151	OCS	OD2-SG-CB	2.58	109.85	105.74
1	C	151	OCS	OD3-SG-CB	2.41	109.81	106.94
1	C	151	OCS	OD2-SG-CB	2.33	109.45	105.74
1	D	151	OCS	OD1-SG-CB	2.28	109.65	106.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	151	OCS	CA-CB-SG-OD1
1	B	151	OCS	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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	B	402	-	5,5,5	0.91	0	5,5,5	1.00	0
2	GOL	B	401	-	5,5,5	0.92	0	5,5,5	0.97	0
2	GOL	D	401	-	5,5,5	0.93	0	5,5,5	0.94	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	B	402	-	-	0/4/4/4	-
2	GOL	B	401	-	-	0/4/4/4	-
2	GOL	D	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	GOL	O1-C1-C2-C3
2	D	401	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	326/335 (97%)	0.71	22 (6%) 17 15	31, 42, 78, 147	0
1	B	324/335 (96%)	0.74	29 (8%) 9 7	31, 42, 81, 150	0
1	C	327/335 (97%)	1.02	56 (17%) 1 1	29, 59, 104, 166	0
1	D	324/335 (96%)	1.09	64 (19%) 1 0	34, 56, 93, 188	0
All	All	1301/1340 (97%)	0.89	171 (13%) 3 2	29, 48, 96, 188	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	182	ALA	8.6
1	D	113	ALA	8.3
1	C	192	HIS	8.0
1	A	191	SER	7.2
1	A	190	PRO	6.3
1	D	238	ASP	6.2
1	D	192	HIS	6.2
1	C	66	LEU	5.9
1	A	64	ASP	5.7
1	D	191	SER	5.4
1	C	29	VAL	5.2
1	C	333	ALA	5.1
1	C	77	GLN	5.0
1	C	113	ALA	4.9
1	A	67	VAL	4.6
1	A	23	GLY	4.5
1	D	91	VAL	4.5
1	B	64	ASP	4.4
1	A	192	HIS	4.3
1	C	48	TYR	4.3
1	D	53	GLY	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	89	SER	4.2
1	C	84	ILE	4.2
1	B	238	ASP	4.1
1	A	1	MET	4.0
1	C	211	GLY	3.9
1	D	55	TYR	3.8
1	B	50	SER	3.8
1	B	67	VAL	3.8
1	C	67	VAL	3.8
1	B	63	GLY	3.7
1	B	55	TYR	3.7
1	D	62	SER	3.7
1	B	73	ILE	3.6
1	A	73	ILE	3.5
1	B	71	HIS	3.5
1	C	91	VAL	3.5
1	C	49	ASP	3.4
1	C	183	THR	3.4
1	C	14	GLY	3.4
1	D	54	ARG	3.4
1	B	30	VAL	3.4
1	C	64	ASP	3.3
1	D	2	ALA	3.3
1	C	28	GLU	3.3
1	C	317	TYR	3.2
1	D	3	ILE	3.2
1	A	46	PHE	3.2
1	D	48	TYR	3.2
1	D	6	GLY	3.2
1	D	123	PRO	3.2
1	B	1	MET	3.1
1	C	181	THR	3.1
1	D	60	THR	3.1
1	D	59	VAL	3.1
1	C	73	ILE	3.1
1	D	1	MET	3.1
1	C	314	ASP	3.1
1	C	224	ASN	3.0
1	C	76	PHE	3.0
1	B	126	ASP	3.0
1	C	193	LYS	3.0
1	D	50	SER	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	31	ALA	2.9
1	C	106	GLY	2.9
1	D	30	VAL	2.9
1	D	325	ASP	2.9
1	D	89	SER	2.9
1	D	124	SER	2.9
1	A	3	ILE	2.8
1	B	66	LEU	2.8
1	C	90	GLY	2.8
1	D	20	VAL	2.8
1	B	51	THR	2.8
1	B	70	GLY	2.8
1	D	63	GLY	2.8
1	C	42	ALA	2.8
1	D	272	VAL	2.8
1	A	220	ILE	2.8
1	D	115	ALA	2.8
1	D	193	LYS	2.8
1	D	203	GLY	2.8
1	B	36	PHE	2.7
1	A	335	ALA	2.7
1	C	120	ILE	2.7
1	A	181	THR	2.7
1	B	191	SER	2.7
1	D	137	ASP	2.7
1	B	317[A]	TYR	2.7
1	D	22	LEU	2.6
1	D	36	PHE	2.6
1	D	4	LYS	2.6
1	D	90	GLY	2.6
1	C	115	ALA	2.6
1	C	83	ASN	2.6
1	D	134	VAL	2.6
1	D	45	MET	2.6
1	D	94	VAL	2.5
1	C	162	VAL	2.5
1	D	51	THR	2.5
1	C	43	ALA	2.5
1	C	118	VAL	2.5
1	D	64	ASP	2.5
1	D	99	GLY	2.4
1	B	220	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	100	VAL	2.4
1	D	29	VAL	2.4
1	A	299	GLY	2.4
1	D	317	TYR	2.4
1	C	335	ALA	2.4
1	D	157	ALA	2.4
1	A	91	VAL	2.4
1	C	63	GLY	2.4
1	C	75	VAL	2.4
1	B	9	GLY	2.4
1	B	76	PHE	2.4
1	D	223	LEU	2.3
1	C	54	ARG	2.3
1	D	26	ASP	2.3
1	D	254	TYR	2.3
1	B	140	THR	2.3
1	A	58[A]	GLU	2.3
1	D	40	ASP	2.3
1	C	57	GLY	2.3
1	C	108	GLN	2.3
1	D	81	PRO	2.3
1	D	68	ILE	2.3
1	C	228	THR	2.2
1	A	63	GLY	2.2
1	D	9	GLY	2.2
1	B	54	ARG	2.2
1	D	27	ILE	2.2
1	A	71	HIS	2.2
1	A	203	GLY	2.2
1	C	110	HIS	2.2
1	D	65	ASP	2.2
1	D	87	GLY	2.2
1	A	317[A]	TYR	2.2
1	D	93	TYR	2.2
1	C	8	ASN	2.2
1	D	97	SER	2.2
1	C	35	PRO	2.2
1	B	53	GLY	2.2
1	D	70	GLY	2.2
1	D	76	PHE	2.2
1	D	249	LYS	2.2
1	C	55	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	67	VAL	2.1
1	B	52	HIS	2.1
1	D	92	ASP	2.1
1	C	1	MET	2.1
1	C	102	THR	2.1
1	B	194	ASP	2.1
1	B	37	ILE	2.1
1	A	238	ASP	2.1
1	C	19	ARG	2.1
1	C	293	ILE	2.1
1	B	192	HIS	2.1
1	C	71	HIS	2.1
1	C	111	ILE	2.1
1	D	42	ALA	2.1
1	B	88	LYS	2.1
1	C	134	VAL	2.0
1	A	65	ASP	2.0
1	C	265	SER	2.0
1	D	75	VAL	2.0
1	C	112[A]	ASP	2.0
1	D	194	ASP	2.0
1	D	327	LEU	2.0
1	B	208	SER	2.0
1	C	170	GLU	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	OCS	A	151	8/10	0.88	0.24	36,38,44,49	2
1	OCS	B	151	8/10	0.88	0.20	45,50,54,54	1
1	OCS	D	151	9/10	0.93	0.17	40,44,49,49	2
1	OCS	C	151	9/10	0.96	0.21	38,40,44,47	2

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GOL	B	401	6/6	0.68	0.17	57,60,66,67	0
2	GOL	B	402	6/6	0.79	0.28	49,56,62,63	0
2	GOL	D	401	6/6	0.84	0.19	45,46,47,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.