



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:15 AM UTC

PDB ID : 1GML / pdb_00001gml
Title : crystal structure of the mouse CCT gamma apical domain (triclinic)
Authors : Pappenberger, G.; Wilsher, J.A.; Roe, S.M.; Willison, K.R.; Pearl, L.H.
Deposited on : 2001-09-17
Resolution : 2.20 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

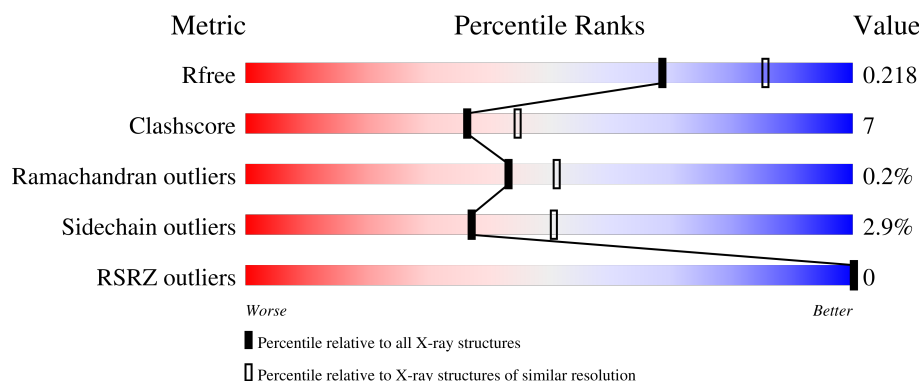
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	178	 74% 13% 13%
1	B	178	 72% 13% 14%
1	C	178	 65% 20% 13%
1	D	178	 63% 19% 16%

2 Entry composition [i](#)

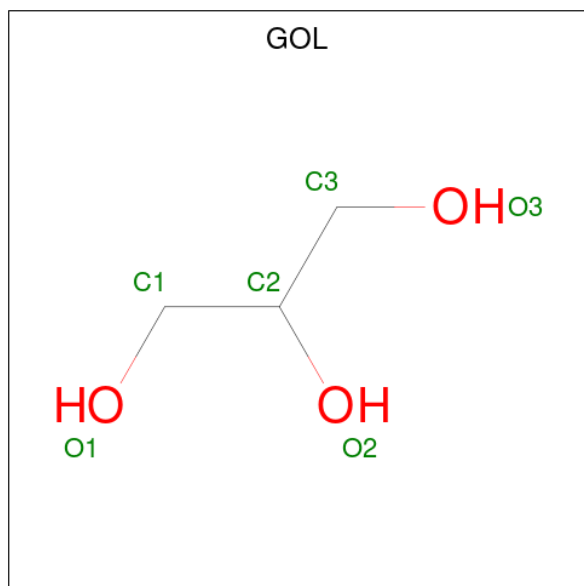
There are 3 unique types of molecules in this entry. The entry contains 5484 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 T-COMPLEX PROTEIN 1 SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	1
			1221	765	221	226	9			
1	B	153	Total	C	N	O	S	0	0	1
			1214	761	219	226	8			
1	C	155	Total	C	N	O	S	0	0	1
			1214	758	219	228	9			
1	D	149	Total	C	N	O	S	0	0	1
			1166	726	217	215	8			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total	O	0	0
			174	174		
3	B	181	Total	O	0	0
			181	181		
3	C	148	Total	O	0	0
			148	148		
3	D	142	Total	O	0	0
			142	142		

● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

K363	K211	G212	G213	R216	K222	R231	Y232	I233	R237	R248	LYS	GLY	GLU	SER	GLN	THR	ASP	ILE	ILE	THR	ARG	GLU	GLU	D263	F264	T265	Q269	L278	D288	V289	V290	Q301	M305	V309	R314	V332	E336	H337	L338	G346	T352
HIS	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	GLU	GLU	SER	GLN	THR	ASP	ILE	ILE	THR	ARG	GLU	GLU	D263	F264	T265	Q269	L278	D288	V289	V290	Q301	M305	V309	R314	V332	E336	H337	L338	G346	T352

● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

E368
T364
G378
A379 SER
HIS
HIS
HIS
HIS
HIS
HIS
HIS

MET
GLU
ASP
SER
CYS
V214
K222
T226
I233
R237
K248
LYS
GLY
GLU
SER
GLN
THR
ASP
ILE
GLU
ILE
THR
ARG
GLU
E262
D263
F264
T265
R266
K269
N270
L278
D288
Q301
P305
R314
V332
E336
E337
L338
G346
I352
K353
K354

● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

RET	G211	T225	H226	P227	A228	H229	L238	G239	L240	P247	G248	LYS	GLY	GLU	SER	GLN	THR	ILE	ILE	GLU	THR	ARG	GLU	GLU	G263	R266	L267	L268	Q269	A270	E271	E272	E273	L278	L285	D288	L291	L296	Q301	M305	A311	L312	R313	L323
A329	R334	P335	E336	E337	L338	G346	L349	L350	E358	L363	K367	L368	P369	L374	R377	G378	A379	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	R286	L287	L288	Q289	A270	E271	E272	E273	L278	L285	D288	L291	L296	Q301	M305	A311	L312	R313	L323

● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

MET	L212	L238	L248	L268	L278	L285	D288	I291	I296	Q301	M305	A311	I323	I326
GLU	S213	V239	K245	GLY	L279	L286	D289	I292	I297	Q302	M306	A312	I324	I327
ASP	V214	L240	L246	GLY	L280	L287	D290	I293	I298	Q303	M307	A313	I325	I328
L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229
H226	H227	H228	H229	H230	H231	H232	H233	H234	H235	H236	H237	H238	H239	H240
R228	R229	R230	R231	R232	R233	R234	R235	R236	R237	R238	R239	R240	R241	R242
M229	M230	M231	M232	M233	M234	M235	M236	M237	M238	M239	M240	M241	M242	M243
N234	N235	N236	N237	N238	N239	N240	N241	N242	N243	N244	N245	N246	N247	N248
I238	I239	I240	I241	I242	I243	I244	I245	I246	I247	I248	I249	I250	I251	I252
V239	V240	V241	V242	V243	V244	V245	V246	V247	V248	V249	V250	V251	V252	V253
L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254
K245	K246	K247	K248	K249	K250	K251	K252	K253	K254	K255	K256	K257	K258	K259
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282
L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292
L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299
D288	D289	D290	D291	D292	D293	D294	D295	D296	D297	D298	D299	D300	D301	D302
I291	I292	I293	I294	I295	I296	I297	I298	I299	I300	I301	I302	I303	I304	I305
I296	I297	I298	I299	I300	I301	I302	I303	I304	I305	I306	I307	I308	I309	I310
Q301	Q302	Q303	Q304	Q305										

R325	A326	A329	R334	P335	E336	E337	L338	G346	L349	L350	E358	I363	K367	D368	P369	I374	R377	G378	A379	SER	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.74Å 65.02Å 65.47Å 89.97° 103.95° 90.35°	Depositor
Resolution (Å)	28.95 – 2.20 28.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.9 (28.95-2.20) 93.0 (28.95-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.72 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.234 0.184 , 0.218	Depositor DCC
R_{free} test set	1862 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	1.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.084 for -h,k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5484	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.99% 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

5.1 Standard geometry

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	0.63	1/1235 (0.1%)	0.99	7/1663 (0.4%)
1	B	0.63	1/1228 (0.1%)	0.99	7/1653 (0.4%)
1	C	0.59	1/1228 (0.1%)	0.96	3/1657 (0.2%)
1	D	0.58	1/1179 (0.1%)	0.97	4/1589 (0.3%)
All	All	0.61	4/4870 (0.1%)	0.98	21/6562 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	378	GLY	C-N	-5.50	1.25	1.33
1	D	378	GLY	C-N	-5.45	1.25	1.33
1	A	378	GLY	C-N	-5.26	1.25	1.33
1	B	378	GLY	C-N	-5.24	1.26	1.33

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	238	ILE	N-CA-C	6.66	117.49	108.17
1	D	238	ILE	N-CA-C	6.58	117.38	108.17
1	A	288	ASP	N-CA-C	-6.02	106.06	113.41
1	B	288	ASP	N-CA-C	-5.99	106.11	113.41
1	C	358	GLU	N-CA-C	5.61	118.83	110.14

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	1221	0	1242	14	0
1	B	1214	0	1239	15	0
1	C	1214	0	1218	22	0
1	D	1166	0	1181	20	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	A	174	0	0	7	0
3	B	181	0	0	5	0
3	C	148	0	0	0	0
3	D	142	0	0	0	0
All	All	5484	0	4912	70	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 7.

The worst 5 of 70 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:301:GLN:HG2	1:A:305:MET:HE2	1.37	1.04
1:B:301:GLN:HG2	1:B:305:MET:HE2	1.37	1.03
1:B:262:GLU:HG2	1:B:263:ASP:H	1.38	0.88
1:D:285:LEU:HD11	1:D:338:LEU:HB3	1.65	0.78
1:C:285:LEU:HD11	1:C:338:LEU:HB3	1.66	0.78

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	151/178 (85%)	149 (99%)	2 (1%)	0	100	100
1	B	149/178 (84%)	146 (98%)	2 (1%)	1 (1%)	18	19
1	C	151/178 (85%)	147 (97%)	4 (3%)	0	100	100
1	D	145/178 (82%)	140 (97%)	5 (3%)	0	100	100
All	All	596/712 (84%)	582 (98%)	13 (2%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	ASP

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	133/160 (83%)	131 (98%)	2 (2%)	57	73
1	B	133/160 (83%)	131 (98%)	2 (2%)	57	73
1	C	132/160 (82%)	126 (96%)	6 (4%)	24	33
1	D	126/160 (79%)	121 (96%)	5 (4%)	28	38
All	All	524/640 (82%)	509 (97%)	15 (3%)	37	51

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	336	GLU
1	D	349	LEU
1	C	349	LEU
1	D	350	LEU
1	D	325	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	321	ASN
1	D	221	ASN
1	D	235	ASN
1	B	235	ASN
1	B	301	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	A	1379	-	5,5,5	0.47	0	5,5,5	0.74	0
2	GOL	C	1379	-	5,5,5	0.55	0	5,5,5	0.67	0
2	GOL	B	1379	-	5,5,5	0.51	0	5,5,5	0.68	0
2	GOL	D	1379	-	5,5,5	0.50	0	5,5,5	0.66	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	A	1379	-	-	4/4/4/4	-
2	GOL	C	1379	-	-	1/4/4/4	-
2	GOL	B	1379	-	-	0/4/4/4	-
2	GOL	D	1379	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1379	GOL	O1-C1-C2-C3
2	A	1379	GOL	C1-C2-C3-O3
2	C	1379	GOL	C1-C2-C3-O3
2	A	1379	GOL	O2-C2-C3-O3
2	A	1379	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, 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	155/178 (87%)	-1.62	0 100 100	26, 35, 58, 88	0
1	B	153/178 (85%)	-1.63	0 100 100	26, 35, 55, 88	0
1	C	155/178 (87%)	-1.61	0 100 100	27, 39, 68, 84	0
1	D	149/178 (83%)	-1.62	0 100 100	27, 39, 74, 99	0
All	All	612/712 (85%)	-1.62	0 100 100	26, 37, 66, 99	0

There are no RSRZ outliers to report.

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 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(Å ²)	Q<0.9
2	GOL	A	1379	6/6	0.99	0.03	33,46,51,53	0
2	GOL	B	1379	6/6	0.99	0.04	39,52,58,62	0
2	GOL	C	1379	6/6	0.99	0.03	39,54,58,63	0
2	GOL	D	1379	6/6	0.99	0.03	41,43,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.