



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:34 PM UTC

PDB ID : 3L19 / pdb_00003l19
Title : Crystal structure of calcium binding domain of CpCDPK3, cgd5_820
Authors : Qiu, W.; Hutchinson, A.; Wernimont, A.; Walker, J.R.; Sullivan, H.; Lin, Y.-H.; Mackenzie, F.; Kozieradzki, I.; Cossar, D.; Schapira, M.; Senisterra, G.; Vedadi, M.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Bochkarev, A.; Hui, R.; Amani, M.; Structural Genomics Consortium (SGC)
Deposited on : 2009-12-11
Resolution : 2.14 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

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

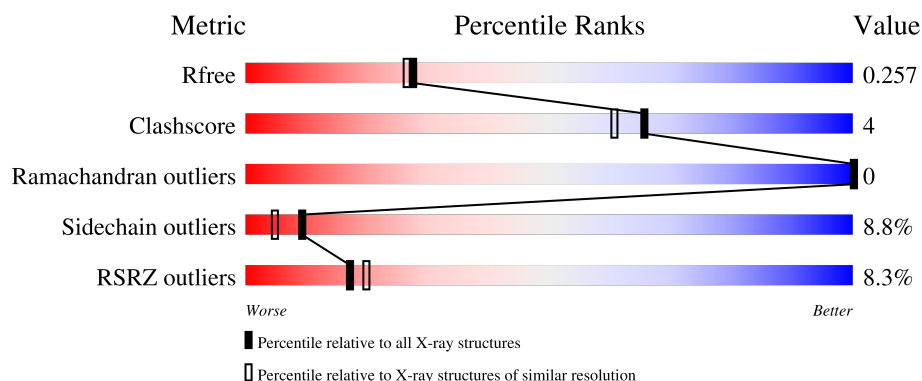
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	214	6% 74% 10% • 14%
1	B	214	8% 72% 10% • 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3052 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 Calcium/calmodulin dependent protein kinase with a kinase domain and 4 calmodulin like EF hands.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1451	905	237	302	7			
1	B	179	Total	C	N	O	S	0	1	0
			1421	887	232	294	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	MET	-	expression tag	UNP Q5CS01
A	308	HIS	-	expression tag	UNP Q5CS01
A	309	HIS	-	expression tag	UNP Q5CS01
A	310	HIS	-	expression tag	UNP Q5CS01
A	311	HIS	-	expression tag	UNP Q5CS01
A	312	HIS	-	expression tag	UNP Q5CS01
A	313	HIS	-	expression tag	UNP Q5CS01
A	314	SER	-	expression tag	UNP Q5CS01
A	315	SER	-	expression tag	UNP Q5CS01
A	316	GLY	-	expression tag	UNP Q5CS01
A	317	ARG	-	expression tag	UNP Q5CS01
A	318	GLU	-	expression tag	UNP Q5CS01
A	319	ASN	-	expression tag	UNP Q5CS01
A	320	LEU	-	expression tag	UNP Q5CS01
A	321	TYR	-	expression tag	UNP Q5CS01
A	322	PHE	-	expression tag	UNP Q5CS01
A	323	GLN	-	expression tag	UNP Q5CS01
A	324	GLY	-	expression tag	UNP Q5CS01
B	307	MET	-	expression tag	UNP Q5CS01
B	308	HIS	-	expression tag	UNP Q5CS01
B	309	HIS	-	expression tag	UNP Q5CS01
B	310	HIS	-	expression tag	UNP Q5CS01
B	311	HIS	-	expression tag	UNP Q5CS01
B	312	HIS	-	expression tag	UNP Q5CS01

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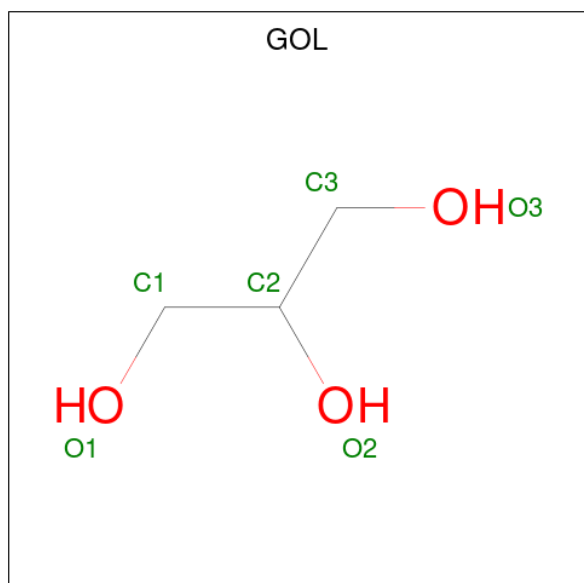
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Chain	Residue	Modelled	Actual	Comment	Reference
B	313	HIS	-	expression tag	UNP Q5CS01
B	314	SER	-	expression tag	UNP Q5CS01
B	315	SER	-	expression tag	UNP Q5CS01
B	316	GLY	-	expression tag	UNP Q5CS01
B	317	ARG	-	expression tag	UNP Q5CS01
B	318	GLU	-	expression tag	UNP Q5CS01
B	319	ASN	-	expression tag	UNP Q5CS01
B	320	LEU	-	expression tag	UNP Q5CS01
B	321	TYR	-	expression tag	UNP Q5CS01
B	322	PHE	-	expression tag	UNP Q5CS01
B	323	GLN	-	expression tag	UNP Q5CS01
B	324	GLY	-	expression tag	UNP Q5CS01

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Ca 4 4	0	0
2	B	4	Total Ca 4 4	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



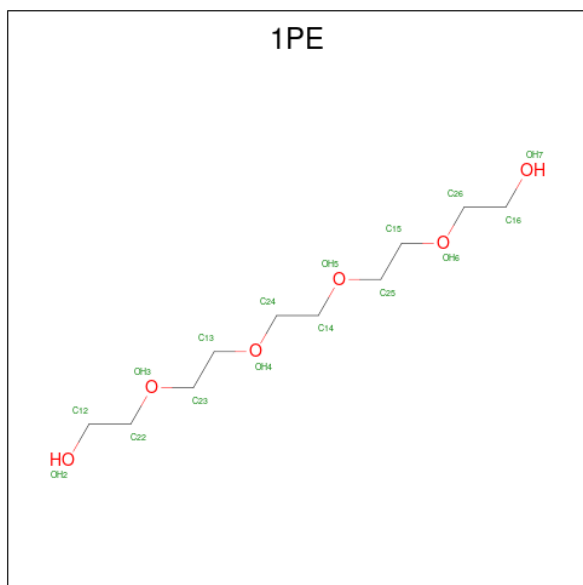
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

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

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	8	5		

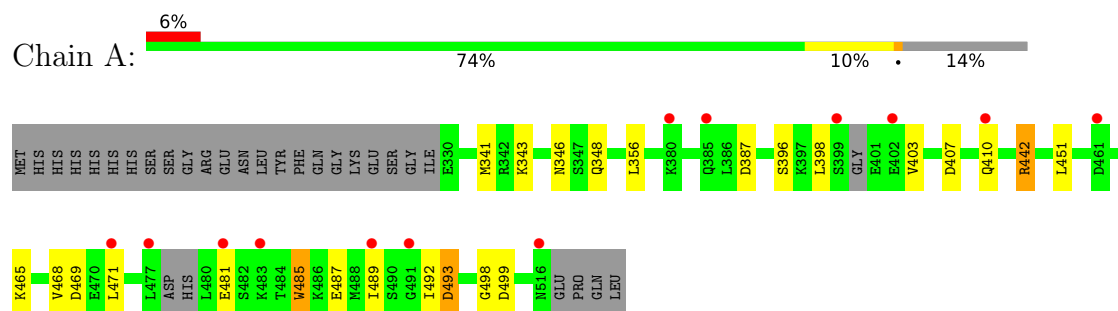
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	B	73	Total	O	0	0
			73	73		

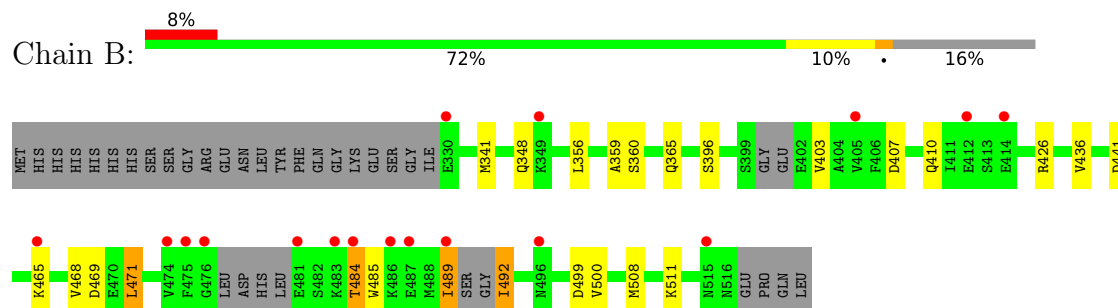
3 Residue-property plots [i](#)

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: Calcium/calmodulin dependent protein kinase with a kinase domain and 4 calmodulin like EF hands



- Molecule 1: Calcium/calmodulin dependent protein kinase with a kinase domain and 4 calmodulin like EF hands



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.57Å 64.19Å 72.81Å 90.00° 97.86° 90.00°	Depositor
Resolution (Å)	19.35 – 2.14 19.35 – 2.14	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.35-2.14) 97.6 (19.35-2.14)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.15Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.215 , 0.257 (Not available) , 0.257	Depositor DCC
R_{free} test set	1168 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3052	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0137e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 1PE, GOL, CA

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	0.89	1/1467 (0.1%)	1.30	3/1966 (0.2%)
1	B	0.83	0/1439	1.32	3/1926 (0.2%)
All	All	0.86	1/2906 (0.0%)	1.31	6/3892 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	LEU	C-N	-8.80	1.21	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	THR	N-CA-C	-9.69	101.15	113.16
1	B	484	THR	CA-C-N	7.53	130.37	120.28
1	B	484	THR	C-N-CA	7.53	130.37	120.28
1	A	492	ILE	N-CA-C	-5.92	106.94	111.62
1	A	387	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	493	ASP	CA-CB-CG	5.03	117.63	112.60

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	1451	0	1404	11	0
1	B	1421	0	1376	11	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	6	0	8	0	0
3	B	18	0	24	1	0
4	B	13	0	17	2	0
5	A	62	0	0	0	0
5	B	73	0	0	0	0
All	All	3052	0	2829	22	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 4.

All (22) 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:489:ILE:HG22	1:A:493:ASP:HB2	1.59	0.84
1:A:346:ASN:HD22	1:A:487:GLU:HG3	1.52	0.75
1:B:360:SER:HB2	4:B:1:1PE:H122	1.73	0.69
1:A:343:LYS:HA	1:A:487:GLU:HB2	1.75	0.68
1:A:489:ILE:CG2	1:A:493:ASP:HB2	2.30	0.62
1:B:489:ILE:HD11	1:B:500:VAL:HG21	1.90	0.54
1:A:485:TRP:CH2	1:A:498:GLY:O	2.62	0.53
1:A:442:ARG:N	1:A:442:ARG:HD2	2.26	0.50
1:A:489:ILE:HG22	1:A:493:ASP:CB	2.38	0.50
1:A:341:MET:HE2	1:A:341:MET:HB3	1.83	0.47
1:A:465:LYS:HB2	1:A:499:ASP:HB3	1.97	0.47
1:B:465:LYS:HB2	1:B:499:ASP:HB3	1.98	0.46
1:B:492:ILE:HD13	1:B:508:MET:HB2	1.97	0.45
1:A:485:TRP:HH2	1:A:498:GLY:O	2.01	0.44
1:B:492:ILE:HD11	1:B:500:VAL:HG13	2.00	0.44
1:B:471:LEU:HG	1:B:485:TRP:CZ3	2.54	0.43
1:A:485:TRP:CZ2	1:A:498:GLY:O	2.73	0.42
1:B:365:GLN:HG2	4:B:1:1PE:H142	2.02	0.42
1:B:426:ARG:HG2	3:B:522:GOL:H31	2.02	0.42
1:B:471:LEU:HG	1:B:485:TRP:HZ3	1.84	0.41
1:B:489:ILE:HD11	1:B:500:VAL:CG2	2.50	0.41
1:B:359:ALA:HB1	1:B:436:VAL:HG12	2.02	0.41

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	178/214 (83%)	177 (99%)	1 (1%)	0	100	100
1	B	172/214 (80%)	170 (99%)	2 (1%)	0	100	100
All	All	350/428 (82%)	347 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	161/187 (86%)	148 (92%)	13 (8%)	11	6
1	B	158/187 (84%)	142 (90%)	16 (10%)	7	3
All	All	319/374 (85%)	290 (91%)	29 (9%)	9	4

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	A	356	LEU
1	A	396	SER
1	A	403	VAL
1	A	407	ASP
1	A	410	GLN
1	A	442	ARG
1	A	451	LEU

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Mol	Chain	Res	Type
1	A	468	VAL
1	A	469	ASP
1	A	471	LEU
1	A	481	GLU
1	A	485	TRP
1	B	341[A]	MET
1	B	341[B]	MET
1	B	348	GLN
1	B	356	LEU
1	B	396	SER
1	B	403	VAL
1	B	407	ASP
1	B	410	GLN
1	B	441	ASP
1	B	468	VAL
1	B	469	ASP
1	B	471	LEU
1	B	484	THR
1	B	489	ILE
1	B	492	ILE
1	B	511	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	GLN
1	A	346	ASN
1	A	385	GLN
1	A	389	GLN
1	A	410	GLN
1	A	460	GLN
1	A	516	ASN
1	B	345	GLN
1	B	377	HIS
1	B	385	GLN
1	B	410	GLN
1	B	460	GLN

5.3.3 RNA ⓘ

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](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
3	GOL	A	521	-	5,5,5	0.23	0	5,5,5	0.58	0
3	GOL	B	2	-	5,5,5	0.69	0	5,5,5	1.24	0
3	GOL	B	521	-	5,5,5	0.65	0	5,5,5	0.44	0
4	1PE	B	1	-	12,12,15	1.01	0	11,11,14	0.88	1 (9%)
3	GOL	B	522	-	5,5,5	0.57	0	5,5,5	0.33	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
3	GOL	A	521	-	-	0/4/4/4	-
3	GOL	B	2	-	-	4/4/4/4	-
3	GOL	B	521	-	-	0/4/4/4	-
4	1PE	B	1	-	-	7/10/10/13	-
3	GOL	B	522	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	1PE	OH3-C23-C13	2.28	120.73	110.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2	GOL	C1-C2-C3-O3
3	B	522	GOL	O1-C1-C2-O2
3	B	522	GOL	O1-C1-C2-C3
3	B	2	GOL	O2-C2-C3-O3
4	B	1	1PE	OH2-C12-C22-OH3
4	B	1	1PE	OH6-C15-C25-OH5
3	B	2	GOL	O1-C1-C2-C3
3	B	522	GOL	C1-C2-C3-O3
4	B	1	1PE	OH4-C13-C23-OH3
3	B	2	GOL	O1-C1-C2-O2
3	B	522	GOL	O2-C2-C3-O3
4	B	1	1PE	C23-C13-OH4-C24
4	B	1	1PE	C12-C22-OH3-C23
4	B	1	1PE	C15-C25-OH5-C14
4	B	1	1PE	OH5-C14-C24-OH4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	1PE	2	0
3	B	522	GOL	1	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

6.1 Protein, DNA and RNA chains

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	184/214 (85%)	0.47	13 (7%)	22 25	25, 51, 73, 90	8 (4%)
1	B	179/214 (83%)	0.55	17 (9%)	14 16	25, 48, 74, 84	14 (7%)
All	All	363/428 (84%)	0.51	30 (8%)	17 20	25, 50, 74, 90	22 (6%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	476	GLY	10.1
1	B	496	ASN	6.0
1	B	330	GLU	5.1
1	A	477	LEU	4.6
1	A	491	GLY	4.4
1	A	385	GLN	4.3
1	B	465	LYS	3.8
1	B	487	GLU	3.5
1	A	471	LEU	3.3
1	B	414	GLU	3.3
1	B	349	LYS	3.0
1	A	489	ILE	2.9
1	B	483	LYS	2.9
1	B	515	ASN	2.8
1	A	481	GLU	2.8
1	A	410	GLN	2.8
1	B	489	ILE	2.7
1	B	481	GLU	2.7
1	B	486	LYS	2.6
1	B	405	VAL	2.6
1	B	474	VAL	2.5
1	A	516	ASN	2.4
1	A	380	LYS	2.3
1	A	461	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	483	LYS	2.3
1	A	402	GLU	2.3
1	B	412	GLU	2.3
1	B	475	PHE	2.1
1	A	399	SER	2.1
1	B	484	THR	2.0

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
3	GOL	B	522	6/6	0.77	0.12	84,86,87,87	0
3	GOL	B	521	6/6	0.78	0.12	64,65,66,67	0
4	1PE	B	1	13/16	0.79	0.19	29,49,87,160	1
3	GOL	B	2	6/6	0.89	0.10	57,58,59,60	0
3	GOL	A	521	6/6	0.94	0.08	64,65,66,68	0
2	CA	A	3	1/1	0.96	0.05	58,58,58,58	0
2	CA	B	4	1/1	0.97	0.06	38,38,38,38	0
2	CA	B	6	1/1	0.97	0.05	46,46,46,46	0
2	CA	B	7	1/1	0.97	0.04	48,48,48,48	0
2	CA	A	1	1/1	0.97	0.04	41,41,41,41	0
2	CA	B	5	1/1	0.98	0.04	41,41,41,41	0
2	CA	A	2	1/1	0.98	0.04	56,56,56,56	0
2	CA	A	8	1/1	0.99	0.03	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.