WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 12, 2017 – 07:19 pm GMT

PDB ID	:	1VAQ
Title	:	Crystal structure of the Mg2+-(chromomycin A3)2-d(TTGGCCAA)2 complex reveals GGCC binding specificity of the drug dimer chelated by metal ion
Authors	:	Hou, M.H.; Robinson, H.; Gao, Y.G.; Wang, A.H.-J.
Deposited on	:	2004-02-19
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

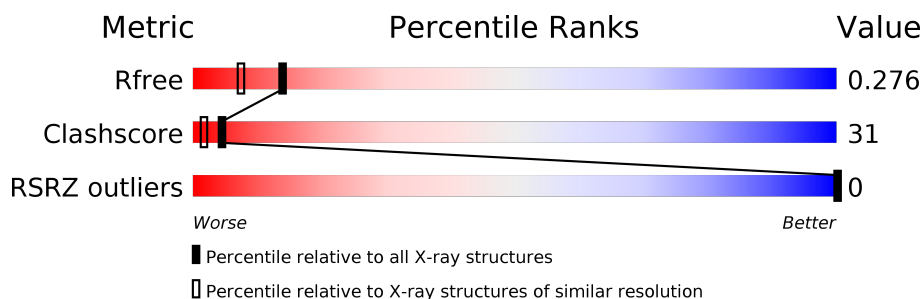|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.00 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	Percentile Ranks	Value
Rfree		0.276
Clashscore		31
RSRZ outliers		0

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	8	25% 63% 13%
1	B	8	38% 25% 25% 13%
1	C	8	13% 50% 25% 13%
1	D	8	38% 38% 25%

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
5	CPH	A	33	-	-	-	X
5	CPH	B	23	-	-	-	X
5	CPH	D	63	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 1261 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 DNA chain called 5'-D(*TP*TP*GP*GP*CP*CP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			
1	B	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			
1	C	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			
1	D	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	2	Total	C	O	0	0
			23	15	8		
2	A	2	Total	C	O	0	0
			23	15	8		
2	D	2	Total	C	O	0	0
			23	15	8		
2	C	2	Total	C	O	0	0
			23	15	8		

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	3	Total	C	O	0	0
			32	21	11		
3	B	3	Total	C	O	0	0
			32	21	11		
3	D	3	Total	C	O	0	0
			32	21	11		
3	C	3	Total	C	O	0	0
			32	21	11		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0

- Molecule 5 is 1,8-DIHYDROXY-7-METHYL-3-(1,3,4-TRIHYDROXY-2-OXO-PENTYL)-3 ,10-DIHYDRO-2H-ANTHRACEN-9-ONE (three-letter code: CPH) (formula: $C_{21}H_{24}O_9$).
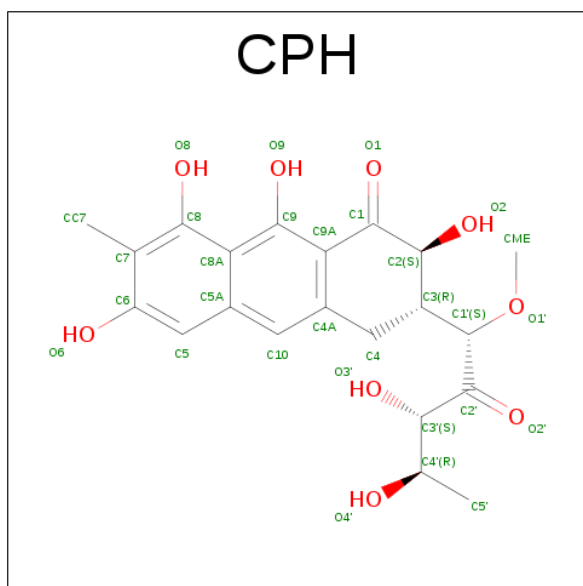
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 28	C 21	O 7	0	0
5	A	1	Total 28	C 21	O 7	0	0
5	D	1	Total 28	C 21	O 7	0	0
5	C	1	Total 28	C 21	O 7	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	33	Total 33	O 33	0	0
6	B	100	Total 100	O 100	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	78	Total O 78 78		0	0
6	D	72	Total O 72 72		0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: 5'-D(*TP*TP*GP*GP*CP*CP*AP*A)-3'

Chain A:
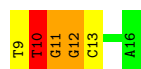
25%　　　　63%　　　　13%

T1 T2 G3 G4 C5 C6 A7 A8

- Molecule 1: 5'-D(*TP*TP*GP*GP*CP*CP*AP*A)-3'

Chain B:

38%　　　25%　　　25%　　13%

T9 T10 G11 G12 C13 A16

- Molecule 1: 5'-D(*TP*TP*GP*GP*CP*CP*AP*A)-3'

Chain C:

13%　　　50%　　　25%　　13%

T41 T42 G43 G44 C45 C46 A47 A48

- Molecule 1: 5'-D(*TP*TP*GP*GP*CP*CP*AP*A)-3'

Chain D:

38%　　　38%　　　25%

T49 T50 G51 G52 C53 C54 A55 A56
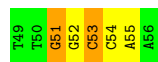
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	42.23Å 42.23Å 246.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.00 19.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.00) 79.8 (19.97-2.00)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.278 0.244 , 0.276	Depositor DCC
R_{free} test set	823 reflections (10.66%)	DCC
Wilson B-factor (Å^2)	15.1	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 102.1	EDS
L-test for twinning[1]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	1261	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Theoretical values of $< |L| >$, $< L^2 >$ 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: CPH, MG, 1GL, CDR, ARI, ERI

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	1.05	0/180	1.35	0/276
1	B	1.16	0/180	1.37	3/276 (1.1%)
1	C	1.11	0/180	1.28	2/276 (0.7%)
1	D	1.08	1/180 (0.6%)	1.30	1/276 (0.4%)
All	All	1.10	1/720 (0.1%)	1.33	6/1104 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	2
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	51	DG	C2-N2	-5.77	1.28	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	DC	O4'-C1'-N1	6.18	112.33	108.00
1	B	10	DT	C5'-C4'-C3'	-5.91	103.47	114.10
1	C	47	DA	O5'-P-OP2	-5.49	100.76	105.70
1	B	10	DT	N1-C1'-C2'	-5.33	102.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	11	DG	N9-C1'-C2'	-5.18	102.77	112.60
1	D	51	DG	N9-C1'-C2'	-5.03	103.04	112.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	DG	Sidechain
1	A	4	DG	Sidechain
1	B	10	DT	Sidechain
1	B	11	DG	Sidechain
1	B	12	DG	Sidechain
1	C	44	DG	Sidechain
1	C	45	DC	Sidechain
1	D	51	DG	Sidechain
1	D	53	DC	Sidechain

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	161	0	92	9	0
1	B	161	0	92	6	0
1	C	161	0	92	14	0
1	D	161	0	90	5	0
2	A	23	0	25	1	0
2	B	23	0	25	0	0
2	C	23	0	25	0	0
2	D	23	0	25	1	0
3	B	64	0	66	1	0
3	C	32	0	33	2	0
3	D	32	0	33	3	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	28	0	20	3	0
5	B	28	0	20	6	0
5	C	28	0	20	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	28	0	20	4	0
6	A	33	0	0	2	0
6	B	100	0	0	4	0
6	C	78	0	0	10	0
6	D	72	0	0	3	0
All	All	1261	0	678	52	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 31.

All (52) 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:45:DC:H1'	6:C:230:HOH:O	1.61	0.99
5:B:23:CPH:H5'B	6:B:431:HOH:O	1.69	0.92
1:B:10:DT:H1'	6:B:208:HOH:O	1.75	0.86
1:C:46:DC:H5'	6:C:230:HOH:O	1.77	0.83
1:D:52:DG:H2''	1:D:53:DC:H5'	1.61	0.83
1:C:45:DC:C1'	6:C:230:HOH:O	2.24	0.82
1:B:12:DG:H2''	1:B:13:DC:H5'	1.62	0.80
1:C:46:DC:OP1	5:C:73:CPH:H5'B	1.83	0.78
2:D:61:1GL:H63	6:D:323:HOH:O	1.87	0.75
5:C:73:CPH:H5'A	5:C:73:CPH:H4	1.72	0.71
5:C:73:CPH:H1'	6:C:298:HOH:O	1.93	0.69
5:B:23:CPH:HME	3:C:75:CDR:H21	1.74	0.67
1:C:44:DG:H2''	1:C:45:DC:H5'	1.76	0.67
3:C:75:CDR:H32	5:D:63:CPH:HC7B	1.77	0.67
1:A:1:DT:H2''	1:A:2:DT:H5'	1.79	0.65
1:B:9:DT:H2'	1:B:10:DT:H72	1.79	0.64
1:A:2:DT:H2''	1:A:3:DG:H5'	1.80	0.63
1:D:52:DG:C2'	1:D:53:DC:H5'	2.27	0.63
3:D:65:CDR:H62	6:D:449:HOH:O	2.00	0.62
1:C:46:DC:H2'	1:C:47:DA:C8	2.37	0.59
1:A:6:DC:H5''	5:A:33:CPH:O3'	2.02	0.58
1:B:9:DT:H2'	1:B:10:DT:C7	2.33	0.57
1:C:45:DC:C2'	6:C:230:HOH:O	2.52	0.55
5:C:73:CPH:HC7B	3:D:65:CDR:H32	1.89	0.54
5:B:23:CPH:H5'A	6:B:351:HOH:O	2.06	0.54
1:C:42:DT:H1'	1:C:43:DG:C8	2.43	0.53
1:A:6:DC:H5''	5:A:33:CPH:H3	1.89	0.53
1:A:2:DT:H2''	1:A:3:DG:C5'	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:73:CPH:H5'A	5:C:73:CPH:C4	2.40	0.50
1:C:44:DG:N7	6:C:429:HOH:O	2.35	0.49
5:B:23:CPH:HME	1:C:47:DA:H4'	1.94	0.49
1:A:1:DT:H2"	1:A:2:DT:C5'	2.44	0.48
1:A:1:DT:H2'	1:A:2:DT:H71	1.95	0.48
5:C:73:CPH:H5'	6:C:427:HOH:O	2.12	0.47
5:D:63:CPH:H1'	6:D:315:HOH:O	2.14	0.47
5:A:33:CPH:HC7B	3:B:25:CDR:H32	1.97	0.46
1:D:53:DC:H4'	5:D:63:CPH:C5A	2.45	0.46
2:A:32:ARI:H32	6:A:240:HOH:O	2.16	0.46
1:A:5:DC:N4	6:A:239:HOH:O	2.39	0.46
1:C:43:DG:N7	6:C:222:HOH:O	2.36	0.45
1:C:43:DG:C8	6:C:222:HOH:O	2.70	0.45
3:D:66:ERI:OGL	3:D:66:ERI:H32	2.17	0.45
1:D:54:DC:H2"	1:D:55:DA:H5'	1.98	0.45
1:A:1:DT:H2'	1:A:2:DT:C6	2.51	0.45
1:C:42:DT:C2	1:C:43:DG:N7	2.87	0.43
5:C:73:CPH:HMEB	6:C:298:HOH:O	2.18	0.43
5:B:23:CPH:H5'	1:C:48:DA:OP1	2.19	0.42
5:C:73:CPH:C3	5:C:73:CPH:H5'A	2.49	0.42
1:D:54:DC:OP1	5:D:63:CPH:O2'	2.37	0.42
1:B:9:DT:H2"	1:B:10:DT:O5'	2.19	0.41
1:B:9:DT:C6	1:B:10:DT:H72	2.56	0.41
5:B:23:CPH:C5'	6:B:350:HOH:O	2.68	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

20 carbohydrates 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	1GL	A	31	2	11,11,11	2.13	4 (36%)	12,15,15	2.19	6 (50%)
2	ARI	A	32	2,5	12,12,12	1.90	3 (25%)	15,16,16	2.58	4 (26%)
2	1GL	B	21	2	11,11,11	2.20	6 (54%)	12,15,15	2.59	4 (33%)
2	ARI	B	22	2,5	12,12,12	1.75	2 (16%)	15,16,16	2.43	2 (13%)
3	CDR	B	24	3,5	9,9,9	1.75	1 (11%)	11,12,12	2.10	4 (36%)
3	CDR	B	25	3	9,9,9	2.03	2 (22%)	11,12,12	2.26	6 (54%)
3	ERI	B	26	3	12,12,14	2.15	5 (41%)	15,16,21	2.30	7 (46%)
3	CDR	B	34	3,5	9,9,9	3.22	3 (33%)	11,12,12	2.02	4 (36%)
3	CDR	B	35	3	9,9,9	2.05	2 (22%)	11,12,12	2.48	6 (54%)
3	ERI	B	36	3	12,12,14	2.10	4 (33%)	15,16,21	2.47	6 (40%)
2	1GL	C	71	2	11,11,11	1.96	3 (27%)	12,15,15	2.01	4 (33%)
2	ARI	C	72	2,5	12,12,12	2.03	4 (33%)	15,16,16	2.14	4 (26%)
3	CDR	C	74	3,5	9,9,9	3.03	2 (22%)	11,12,12	1.98	4 (36%)
3	CDR	C	75	3	9,9,9	1.64	1 (11%)	11,12,12	1.72	2 (18%)
3	ERI	C	76	3	12,12,14	2.02	3 (25%)	15,16,21	2.69	6 (40%)
2	1GL	D	61	2	11,11,11	1.79	3 (27%)	12,15,15	2.57	6 (50%)
2	ARI	D	62	2,5	12,12,12	1.92	2 (16%)	15,16,16	2.28	5 (33%)
3	CDR	D	64	3,5	9,9,9	3.01	3 (33%)	11,12,12	2.08	3 (27%)
3	CDR	D	65	3	9,9,9	2.02	3 (33%)	11,12,12	2.16	6 (54%)
3	ERI	D	66	3	12,12,14	2.31	3 (25%)	15,16,21	2.50	6 (40%)

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	1GL	A	31	2	-	0/2/18/18	0/1/1/1
2	ARI	A	32	2,5	-	0/4/17/17	0/1/1/1
2	1GL	B	21	2	-	0/2/18/18	0/1/1/1
2	ARI	B	22	2,5	-	0/4/17/17	0/1/1/1
3	CDR	B	24	3,5	-	0/0/13/13	0/1/1/1
3	CDR	B	25	3	-	0/0/13/13	0/1/1/1
3	ERI	B	26	3	-	0/16/16/23	0/0/0/1
3	CDR	B	34	3,5	-	0/0/13/13	0/1/1/1
3	CDR	B	35	3	-	0/0/13/13	0/1/1/1
3	ERI	B	36	3	-	0/16/16/23	0/0/0/1
2	1GL	C	71	2	-	0/2/18/18	0/1/1/1
2	ARI	C	72	2,5	-	0/4/17/17	0/1/1/1
3	CDR	C	74	3,5	-	0/0/13/13	0/1/1/1
3	CDR	C	75	3	-	0/0/13/13	0/1/1/1
3	ERI	C	76	3	-	0/16/16/23	0/0/0/1
2	1GL	D	61	2	-	0/2/18/18	0/1/1/1
2	ARI	D	62	2,5	-	0/4/17/17	0/1/1/1
3	CDR	D	64	3,5	-	0/0/13/13	0/1/1/1
3	CDR	D	65	3	-	0/0/13/13	0/1/1/1
3	ERI	D	66	3	-	0/16/16/23	0/0/0/1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	26	ERI	O3-C3	-3.94	1.37	1.44
3	B	26	ERI	C5-C4	2.03	1.60	1.53
2	A	32	ARI	C6-C5	2.05	1.56	1.51
3	C	76	ERI	O4-CO4	2.06	1.39	1.35
2	C	72	ARI	C6-C5	2.07	1.56	1.51
2	D	61	1GL	C2-C1	2.12	1.55	1.51
2	C	72	ARI	O4-C4	2.14	1.49	1.46
3	D	64	CDR	C2-C1	2.14	1.57	1.50
2	B	21	1GL	C2-C3	2.16	1.56	1.52
2	A	31	1GL	C2-C1	2.22	1.55	1.51
3	B	34	CDR	C2-C1	2.23	1.57	1.50
2	B	21	1GL	O5-C5	2.27	1.50	1.44
2	B	21	1GL	O1-C1	2.34	1.44	1.39
2	B	21	1GL	C4-C5	2.34	1.56	1.52
3	B	26	ERI	CME-CO4	2.47	1.58	1.49
3	D	66	ERI	CME-CO4	2.52	1.58	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	65	CDR	C6-C5	2.53	1.57	1.51
3	B	36	ERI	CME-CO4	2.61	1.58	1.49
3	B	35	CDR	C4-C5	2.62	1.57	1.52
2	C	71	1GL	C4-C5	2.70	1.57	1.52
3	B	36	ERI	CC3-C3	2.73	1.57	1.52
2	A	31	1GL	C6-C5	2.76	1.58	1.51
2	D	61	1GL	C4-C5	2.80	1.57	1.52
3	C	76	ERI	CME-CO4	2.82	1.59	1.49
3	C	75	CDR	C4-C5	2.85	1.57	1.52
2	D	62	ARI	CME-CO4	2.89	1.59	1.49
3	D	66	ERI	CC3-C3	2.90	1.57	1.52
3	C	74	CDR	OGL-C1	2.91	1.45	1.39
2	C	72	ARI	CME-CO4	2.92	1.59	1.49
3	B	26	ERI	CC3-C3	2.99	1.58	1.52
3	D	65	CDR	C4-C5	2.99	1.58	1.52
2	C	71	1GL	C3-C4	3.26	1.59	1.52
2	A	31	1GL	C4-C5	3.27	1.58	1.52
2	B	22	ARI	CME-CO4	3.29	1.61	1.49
3	B	34	CDR	C4-C5	3.34	1.58	1.52
3	D	65	CDR	C3-C4	3.41	1.57	1.52
3	B	24	CDR	C3-C4	3.45	1.57	1.52
2	B	21	1GL	C6-C5	3.54	1.60	1.51
2	D	61	1GL	O1-C1	3.66	1.47	1.39
3	B	36	ERI	C2-C1	3.67	1.59	1.52
3	B	25	CDR	C4-C5	3.70	1.59	1.52
3	B	26	ERI	C3-C4	3.73	1.60	1.53
2	C	71	1GL	O1-C1	3.74	1.47	1.39
2	A	32	ARI	C3-C4	3.80	1.60	1.52
2	A	31	1GL	O1-C1	3.80	1.47	1.39
3	B	36	ERI	C3-C4	3.86	1.60	1.53
2	B	22	ARI	C3-C4	3.87	1.60	1.52
2	B	21	1GL	C2-C1	3.94	1.59	1.51
3	B	25	CDR	C3-C4	4.00	1.58	1.52
2	A	32	ARI	CME-CO4	4.32	1.64	1.49
2	D	62	ARI	C3-C4	4.71	1.62	1.52
3	B	35	CDR	C3-C4	4.80	1.59	1.52
3	C	76	ERI	C3-C4	5.15	1.62	1.53
2	C	72	ARI	C3-C4	5.19	1.63	1.52
3	D	64	CDR	C3-C4	5.37	1.60	1.52
3	D	66	ERI	C3-C4	6.33	1.64	1.53
3	D	64	CDR	C4-C5	6.42	1.64	1.52
3	C	74	CDR	C3-C4	7.92	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	34	CDR	C3-C4	8.38	1.65	1.52

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	21	1GL	C6-C5-C4	-5.13	105.45	113.36
3	B	34	CDR	C2-C3-C4	-4.84	104.37	111.83
2	D	61	1GL	C6-C5-C4	-4.83	105.92	113.36
3	D	64	CDR	C2-C3-C4	-4.63	104.69	111.83
3	D	66	ERI	C5-C4-C3	-4.61	106.05	115.18
3	B	24	CDR	C2-C3-C4	-4.55	104.82	111.83
3	B	36	ERI	C5-C4-C3	-4.42	106.42	115.18
3	B	35	CDR	C6-C5-C4	-4.26	105.15	112.76
3	C	74	CDR	C2-C3-C4	-4.11	105.49	111.83
3	B	26	ERI	C5-C4-C3	-3.89	107.47	115.18
2	D	61	1GL	O5-C1-C2	-3.84	107.95	110.77
3	B	25	CDR	C6-C5-C4	-3.83	105.91	112.76
3	C	75	CDR	C2-C3-C4	-3.78	106.00	111.83
2	C	71	1GL	C1-C2-C3	-3.78	104.65	111.13
3	B	35	CDR	C2-C3-C4	-3.76	106.03	111.83
2	A	31	1GL	C6-C5-C4	-3.63	107.77	113.36
3	B	35	CDR	O1-C1-C2	-3.62	108.26	110.78
3	D	65	CDR	C6-C5-C4	-3.54	106.44	112.76
3	B	24	CDR	C6-C5-C4	-3.43	106.63	112.76
2	D	61	1GL	C1-C2-C3	-3.40	105.31	111.13
2	B	21	1GL	O5-C1-C2	-3.33	108.33	110.77
3	C	74	CDR	C6-C5-C4	-3.28	106.90	112.76
3	C	76	ERI	C4-O4-CO4	-3.26	112.84	117.90
3	B	25	CDR	C2-C3-C4	-3.11	107.03	111.83
2	B	21	1GL	C1-C2-C3	-3.11	105.80	111.13
2	A	31	1GL	C1-C2-C3	-3.07	105.87	111.13
3	D	64	CDR	OGL-C1-C2	-3.06	104.30	109.27
2	D	62	ARI	O1-C1-C2	-3.04	108.66	110.78
3	B	34	CDR	C6-C5-C4	-3.00	107.40	112.76
3	B	25	CDR	OGL-C1-C2	-2.92	104.53	109.27
3	C	76	ERI	C5-C4-C3	-2.88	109.47	115.18
3	D	64	CDR	C6-C5-C4	-2.85	107.66	112.76
2	A	32	ARI	O1-C1-C2	-2.85	108.80	110.78
2	C	71	1GL	C6-C5-C4	-2.75	109.12	113.36
3	D	65	CDR	OGL-C1-C2	-2.73	104.84	109.27
2	C	72	ARI	O1-C1-C2	-2.72	108.89	110.78
2	D	61	1GL	O5-C5-C4	-2.70	104.05	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	35	CDR	OGL-C1-C2	-2.69	104.91	109.27
3	C	75	CDR	C6-C5-C4	-2.59	108.13	112.76
3	B	26	ERI	C6-C5-C4	-2.52	106.65	113.19
2	C	71	1GL	O3-C3-C2	-2.51	103.96	110.02
3	D	65	CDR	O1-C5-C4	-2.45	105.58	110.01
3	B	25	CDR	O1-C1-C2	-2.42	109.09	110.78
3	C	74	CDR	O1-C5-C4	-2.38	105.69	110.01
3	D	65	CDR	C2-C3-C4	-2.30	108.28	111.83
2	D	62	ARI	C2-C3-C4	-2.28	106.34	111.04
3	B	26	ERI	O3-C3-C4	-2.25	102.95	108.03
2	D	61	1GL	O3-C3-C2	-2.16	104.80	110.02
3	B	36	ERI	C6-C5-C4	-2.11	107.71	113.19
3	B	24	CDR	OGL-C1-C2	-2.09	105.87	109.27
2	A	31	1GL	O3-C3-C2	-2.06	105.05	110.02
2	A	31	1GL	O5-C1-C2	-2.05	109.27	110.77
3	B	34	CDR	OGL-C1-C2	-2.02	105.99	109.27
3	B	34	CDR	O1-C5-C6	2.01	110.94	106.69
2	C	72	ARI	OGL-C1-C2	2.03	112.56	109.27
2	D	62	ARI	C3-C2-C1	2.03	115.46	110.85
3	C	76	ERI	O3-C3-C2	2.09	111.44	106.79
3	B	35	CDR	OGL-C1-O1	2.09	112.91	108.17
3	D	66	ERI	C4-O4-CO4	2.19	121.30	117.90
3	B	25	CDR	OGL-C1-O1	2.19	113.15	108.17
3	D	65	CDR	OGL-C1-O1	2.22	113.21	108.17
2	A	31	1GL	CME-O4-C4	2.25	120.70	114.54
2	A	32	ARI	OGL-C1-O1	2.35	113.51	108.17
3	C	74	CDR	O1-C5-C6	2.47	111.91	106.69
3	B	24	CDR	O1-C5-C6	2.63	112.26	106.69
3	B	26	ERI	C4-O4-CO4	2.73	122.14	117.90
3	B	25	CDR	O1-C5-C6	2.75	112.50	106.69
3	D	66	ERI	O4-CO4-CME	2.84	116.43	111.10
3	B	35	CDR	O1-C5-C6	2.85	112.73	106.69
3	D	66	ERI	CC3-C3-C4	2.85	117.51	110.68
3	D	65	CDR	O1-C5-C6	3.01	113.06	106.69
3	B	26	ERI	O4-C4-C5	3.09	113.51	107.44
2	C	71	1GL	O5-C5-C6	3.14	113.33	106.69
3	D	66	ERI	O4-C4-C3	3.29	110.75	106.52
2	D	61	1GL	O5-C5-C6	3.30	113.67	106.69
3	B	36	ERI	O4-CO4-CME	3.39	117.47	111.10
3	C	76	ERI	O4-C4-C5	3.42	114.16	107.44
3	B	36	ERI	O4-C4-C5	3.45	114.21	107.44
3	B	26	ERI	O4-C4-C3	3.50	111.01	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	26	ERI	O4-CO4-CME	3.62	117.90	111.10
2	A	31	1GL	O5-C5-C6	3.72	114.55	106.69
3	B	36	ERI	C4-O4-CO4	3.73	123.68	117.90
2	C	72	ARI	O4-CO4-CME	4.05	118.71	111.10
3	C	76	ERI	O4-CO4-CME	4.28	119.13	111.10
3	B	36	ERI	O4-C4-C3	4.31	112.05	106.52
2	D	62	ARI	C4-O4-CO4	4.59	124.75	117.47
2	D	62	ARI	O4-CO4-CME	4.61	119.76	111.10
3	D	66	ERI	O4-C4-C5	4.73	116.72	107.44
2	C	72	ARI	C4-O4-CO4	4.85	125.16	117.47
2	B	21	1GL	O5-C5-C6	4.87	117.00	106.69
2	B	22	ARI	O4-CO4-CME	5.18	120.83	111.10
2	A	32	ARI	C4-O4-CO4	5.47	126.16	117.47
2	A	32	ARI	O4-CO4-CME	5.54	121.50	111.10
3	C	76	ERI	O4-C4-C3	6.23	114.51	106.52
2	B	22	ARI	C4-O4-CO4	6.33	127.52	117.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	32	ARI	1	0
3	B	25	CDR	1	0
3	C	75	CDR	2	0
2	D	61	1GL	1	0
3	D	65	CDR	2	0
3	D	66	ERI	1	0

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
5	CPH	A	33	3,2,4	28,30,32	1.97	7 (25%)	35,45,49	2.31	11 (31%)
5	CPH	B	23	3,2,4	28,30,32	1.71	6 (21%)	35,45,49	2.07	16 (45%)
5	CPH	C	73	3,2,4	28,30,32	2.29	11 (39%)	35,45,49	2.79	9 (25%)
5	CPH	D	63	3,2,4	28,30,32	1.94	9 (32%)	35,45,49	2.78	13 (37%)

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	CPH	A	33	3,2,4	-	1/18/30/34	0/3/3/3
5	CPH	B	23	3,2,4	-	0/18/30/34	0/3/3/3
5	CPH	C	73	3,2,4	-	0/18/30/34	0/3/3/3
5	CPH	D	63	3,2,4	-	0/18/30/34	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	63	CPH	CC7-C7	-2.66	1.45	1.51
5	C	73	CPH	C4-C4A	-2.54	1.47	1.51
5	D	63	CPH	O3'-C3'	-2.30	1.37	1.42
5	B	23	CPH	O3'-C3'	-2.24	1.37	1.42
5	B	23	CPH	C4-C4A	-2.22	1.47	1.51
5	C	73	CPH	C8-C8A	2.05	1.50	1.43
5	D	63	CPH	C9A-C4A	2.05	1.45	1.41
5	A	33	CPH	C5-C6	2.07	1.40	1.36
5	D	63	CPH	C2-C1	2.22	1.54	1.50
5	B	23	CPH	O1-C1	2.23	1.26	1.22
5	C	73	CPH	C9A-C9	2.32	1.43	1.40
5	B	23	CPH	C10-C4A	2.44	1.41	1.37
5	C	73	CPH	O8-C8	2.53	1.44	1.35
5	B	23	CPH	C5-C6	2.66	1.42	1.36
5	D	63	CPH	C10-C4A	2.73	1.42	1.37
5	A	33	CPH	C2-C3	2.80	1.60	1.53
5	C	73	CPH	C5-C6	2.98	1.42	1.36
5	A	33	CPH	C8A-C5A	3.00	1.48	1.42
5	C	73	CPH	C2-C1	3.16	1.56	1.50
5	A	33	CPH	C2-C1	3.22	1.56	1.50
5	D	63	CPH	C9A-C9	3.26	1.44	1.40
5	C	73	CPH	O1-C1	3.65	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	33	CPH	O1'-C1'	3.68	1.49	1.42
5	D	63	CPH	C2-C3	3.69	1.62	1.53
5	C	73	CPH	C10-C4A	3.88	1.44	1.37
5	D	63	CPH	C8A-C5A	3.93	1.50	1.42
5	D	63	CPH	O1'-C1'	4.20	1.51	1.42
5	C	73	CPH	O1'-C1'	4.31	1.51	1.42
5	A	33	CPH	C9A-C9	4.36	1.46	1.40
5	C	73	CPH	C8A-C5A	4.53	1.52	1.42
5	B	23	CPH	C8A-C5A	4.73	1.52	1.42
5	A	33	CPH	C10-C4A	4.78	1.46	1.37
5	C	73	CPH	C2-C3	5.22	1.65	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	73	CPH	C9-C9A-C4A	-5.13	116.54	119.80
5	D	63	CPH	C9-C9A-C4A	-4.91	116.68	119.80
5	A	33	CPH	C9-C9A-C4A	-4.28	117.08	119.80
5	B	23	CPH	C2-C3-C1'	-4.10	103.60	111.15
5	C	73	CPH	C6-C5-C5A	-3.79	114.95	120.83
5	C	73	CPH	C4-C4A-C10	-3.46	115.38	121.15
5	B	23	CPH	C6-C5-C5A	-3.32	115.68	120.83
5	D	63	CPH	C6-C5-C5A	-3.26	115.78	120.83
5	D	63	CPH	C4-C4A-C10	-3.07	116.03	121.15
5	D	63	CPH	C7-C8-C8A	-2.79	115.45	121.39
5	B	23	CPH	C4A-C10-C5A	-2.72	116.50	121.29
5	B	23	CPH	O1-C1-C2	-2.67	116.88	120.74
5	C	73	CPH	C7-C8-C8A	-2.64	115.77	121.39
5	D	63	CPH	C4-C3-C2	-2.46	104.75	110.64
5	D	63	CPH	O1-C1-C2	-2.44	117.22	120.74
5	B	23	CPH	C7-C8-C8A	-2.33	116.42	121.39
5	A	33	CPH	C7-C8-C8A	-2.33	116.44	121.39
5	A	33	CPH	CC7-C7-C6	-2.24	115.91	120.33
5	B	23	CPH	O3'-C3'-C2'	-2.12	107.14	110.86
5	A	33	CPH	C4-C3-C2	-2.07	105.70	110.64
5	B	23	CPH	O9-C9-C9A	-2.03	117.33	121.15
5	B	23	CPH	O8-C8-C7	2.10	125.02	118.92
5	B	23	CPH	C9-C8A-C5A	2.13	120.06	118.20
5	B	23	CPH	C5-C6-C7	2.27	125.29	122.22
5	A	33	CPH	O8-C8-C7	2.29	125.58	118.92
5	B	23	CPH	C8-C8A-C5A	2.34	120.23	118.20
5	B	23	CPH	C2-C1-C9A	2.35	121.56	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	33	CPH	C2-C3-C1'	2.41	115.59	111.15
5	D	63	CPH	C2-C1-C9A	2.52	121.86	117.23
5	D	63	CPH	O8-C8-C7	2.58	126.42	118.92
5	A	33	CPH	C4A-C4-C3	2.59	118.58	112.33
5	B	23	CPH	C4-C3-C1'	2.64	116.03	111.15
5	D	63	CPH	C9-C8A-C5A	2.68	120.53	118.20
5	B	23	CPH	CME-O1'-C1'	2.72	117.86	113.80
5	D	63	CPH	C2-C3-C1'	2.84	116.38	111.15
5	C	73	CPH	C5-C6-C7	2.93	126.17	122.22
5	A	33	CPH	C2-C1-C9A	2.95	122.66	117.23
5	A	33	CPH	C10-C4A-C9A	3.19	123.80	118.41
5	B	23	CPH	C6-C7-C8	3.68	121.45	117.82
5	D	63	CPH	C10-C4A-C9A	3.74	124.71	118.41
5	C	73	CPH	C2-C3-C1'	3.89	118.33	111.15
5	B	23	CPH	C10-C4A-C9A	4.14	125.39	118.41
5	C	73	CPH	C10-C4A-C9A	4.27	125.61	118.41
5	A	33	CPH	C6-C7-C8	4.34	122.11	117.82
5	C	73	CPH	C6-C7-C8	4.41	122.17	117.82
5	D	63	CPH	C6-C7-C8	5.13	122.89	117.82
5	A	33	CPH	CME-O1'-C1'	8.03	125.77	113.80
5	C	73	CPH	CME-O1'-C1'	10.51	129.45	113.80
5	D	63	CPH	CME-O1'-C1'	10.68	129.71	113.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	33	CPH	CME-O1'-C1'-C3

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	33	CPH	3	0
5	B	23	CPH	6	0
5	C	73	CPH	8	0
5	D	63	CPH	4	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(Å²)	Q<0.9
1	A	8/8 (100%)	-0.25	0 100	100	11, 16, 20, 24	0
1	B	8/8 (100%)	-0.32	0 100	100	9, 14, 16, 18	0
1	C	8/8 (100%)	-0.11	0 100	100	12, 13, 28, 29	0
1	D	8/8 (100%)	-0.23	0 100	100	10, 14, 15, 17	0
All	All	32/32 (100%)	-0.23	0 100	100	9, 14, 24, 29	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å²)	Q<0.9
3	ERI	D	66	14/14	0.91	0.14	0.48	4,10,19,23	0
3	CDR	D	64	9/9	0.93	0.13	-	1,11,13,20	0
2	1GL	D	61	11/11	0.94	0.13	-	4,18,27,30	0
3	CDR	C	75	9/9	0.96	0.10	-	3,5,10,13	0
2	1GL	A	31	11/11	0.81	0.20	-	3,24,35,38	0
3	ERI	C	76	14/14	0.95	0.11	-	1,6,13,20	0
3	CDR	D	65	9/9	0.93	0.12	-	3,8,15,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CDR	B	25	9/9	0.94	0.11	-	4,8,14,19	0
3	CDR	B	24	9/9	0.95	0.10	-	3,4,10,12	0
2	ARI	A	32	12/12	0.90	0.15	-	5,13,17,20	0
2	1GL	B	21	11/11	0.91	0.13	-	5,12,17,19	0
2	ARI	D	62	12/12	0.95	0.10	-	3,12,16,18	0
2	ARI	B	22	12/12	0.95	0.10	-	1,13,20,21	0
3	CDR	C	74	9/9	0.93	0.13	-	3,8,18,20	0
3	CDR	B	35	9/9	0.89	0.16	-	5,10,14,15	0
2	1GL	C	71	11/11	0.87	0.19	-	6,13,21,23	0
3	CDR	B	34	9/9	0.94	0.12	-	1,4,13,15	0
2	ARI	C	72	12/12	0.92	0.12	-	4,12,18,20	0
3	ERI	B	36	14/14	0.95	0.13	-	1,9,16,17	0
3	ERI	B	26	14/14	0.92	0.14	-	3,9,16,26	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	CPH	B	23	28/30	0.91	0.15	2.62	1,10,32,39	0
5	CPH	D	63	28/30	0.91	0.15	2.32	1,12,43,52	0
5	CPH	A	33	28/30	0.91	0.17	2.01	4,13,36,59	0
5	CPH	C	73	28/30	0.91	0.15	1.58	2,12,23,49	0
4	MG	D	82	1/1	0.97	0.05	-	9,9,9,9	0
4	MG	A	81	1/1	0.98	0.07	-	5,5,5,5	0

6.5 Other polymers (i)

There are no such residues in this entry.