



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:56 AM EDT

PDB ID : 3E6C / pdb_00003e6c
Title : CprK OCPA DNA Complex
Authors : Levy, C.
Deposited on : 2008-08-15
Resolution : 1.80 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

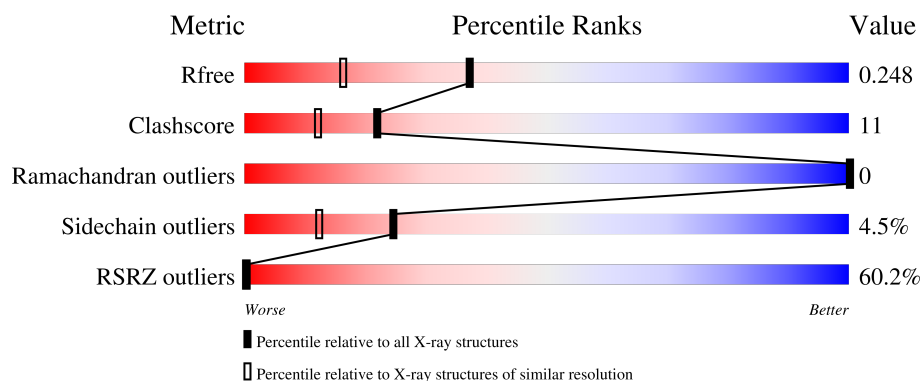
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	C	250	52% 72% 16% 10%
2	B	13	85% 38% 38% 23%
3	A	13	77% 54% 38% 8%

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
4	3C4	C	604	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2506 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 Cyclic nucleotide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	225	Total	C	N	O	S	0	1	0
			1809	1164	296	339	10			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	200	SER	CYS	engineered mutation	UNP Q18R04
C	233	SER	-	expression tag	UNP Q18R04
C	234	ASP	-	expression tag	UNP Q18R04
C	235	PRO	-	expression tag	UNP Q18R04
C	236	ASN	-	expression tag	UNP Q18R04
C	237	SER	-	expression tag	UNP Q18R04
C	238	SER	-	expression tag	UNP Q18R04
C	239	SER	-	expression tag	UNP Q18R04
C	240	VAL	-	expression tag	UNP Q18R04
C	241	ASP	-	expression tag	UNP Q18R04
C	242	LYS	-	expression tag	UNP Q18R04
C	243	LEU	-	expression tag	UNP Q18R04
C	244	ALA	-	expression tag	UNP Q18R04
C	245	ALA	-	expression tag	UNP Q18R04
C	246	ALA	-	expression tag	UNP Q18R04
C	247	LEU	-	expression tag	UNP Q18R04
C	248	ASP	-	expression tag	UNP Q18R04
C	249	HIS	-	expression tag	UNP Q18R04
C	250	HIS	-	expression tag	UNP Q18R04

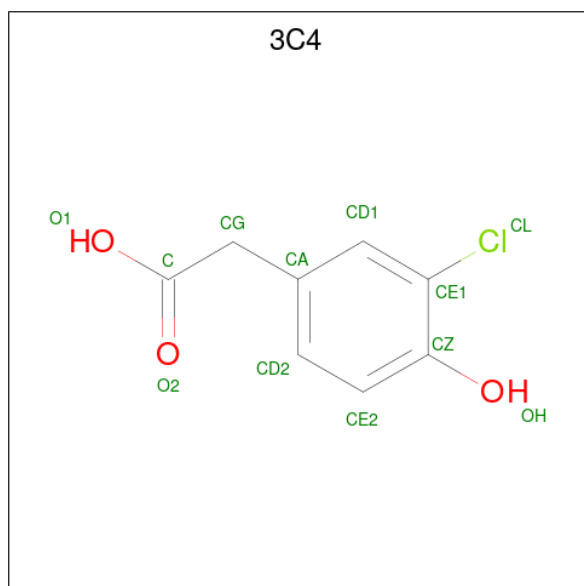
- Molecule 2 is a DNA chain called DNA (5'-D(P*DGP*DCP*DAP*DTP*DTP*DAP*DAP*DCP*DAP*DTP*DGP*DCP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	P	0	0	0
			264	126	48	77	13			

- Molecule 3 is a DNA chain called DNA (5'-D(P*DGP*DGP*DCP*DAP*DTP*DGP*DTP*DTP*DAP*DAP*DTP*DGP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	13	Total	C	N	O	P	0	0	0
			269	128	49	79	13			

- Molecule 4 is (3-CHLORO-4-HYDROXYPHENYL)ACETIC ACID (CCD ID: 3C4) (formula: C₈H₇ClO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	Cl	O	0	0
			12	8	1	3		

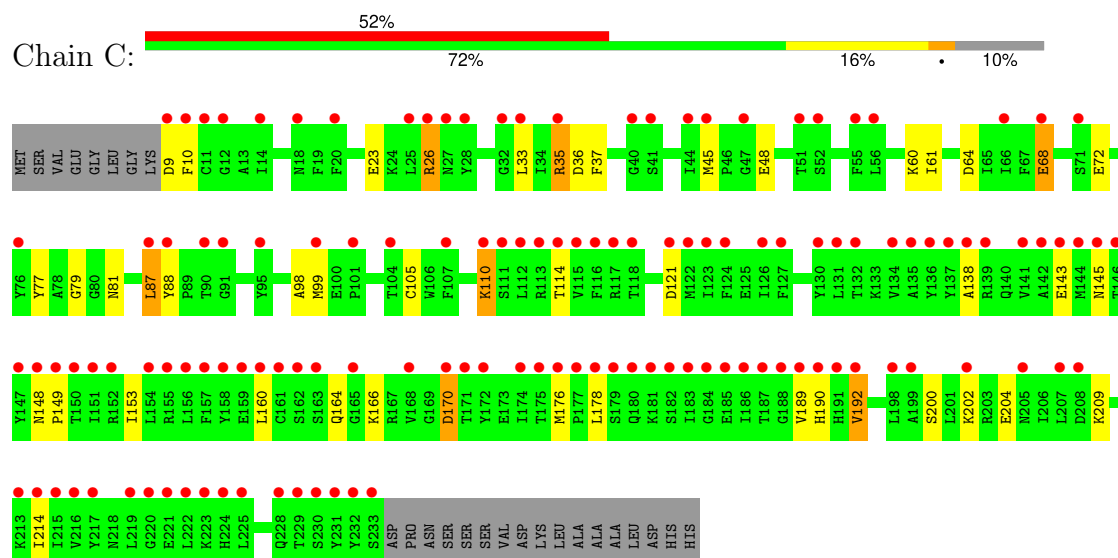
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	136	Total	O	0	0
			136	136		
5	B	6	Total	O	0	0
			6	6		
5	A	10	Total	O	0	0
			10	10		

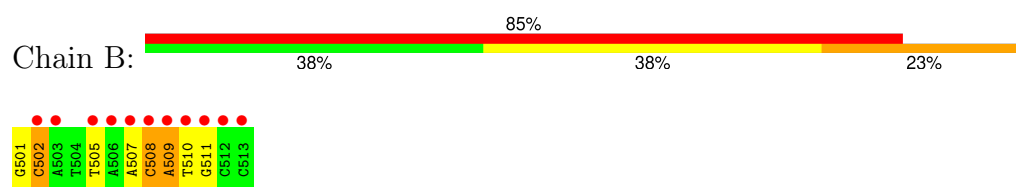
3 Residue-property plots [i](#)

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.

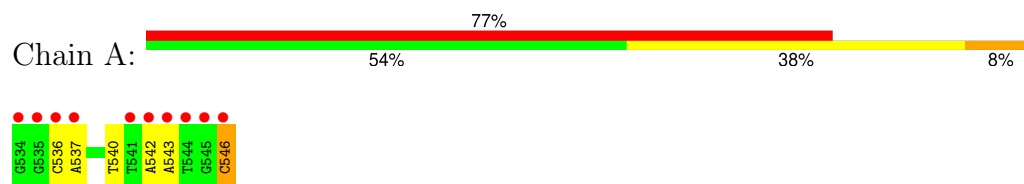
• Molecule 1: Cyclic nucleotide-binding protein



• Molecule 2: DNA (5'-D(P*DGP*DCP*DAP*DTP*DTP*DAP*DAP*DCP*DAP*DTP*DGP*DCP*DC)-3')



• Molecule 3: DNA (5'-D(P*DGP*DGP*DCP*DAP*DTP*DGP*DTP*DTP*DAP*DAP*DTP*DGP*DC)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	100.60Å 100.60Å 149.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.48 – 1.80 27.48 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (27.48-1.80) 99.3 (27.48-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.217 , 0.250 0.221 , 0.248	Depositor DCC
R_{free} test set	2108 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2506	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3C4

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	C	1.47	9/1849 (0.5%)	1.26	6/2495 (0.2%)
2	B	0.71	0/295	1.72	6/452 (1.3%)
3	A	0.61	0/301	1.68	6/463 (1.3%)
All	All	1.32	9/2445 (0.4%)	1.39	18/3410 (0.5%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	36	ASP	C-O	13.25	1.40	1.24
1	C	36	ASP	CG-OD2	8.99	1.42	1.25
1	C	138	ALA	CA-CB	7.82	1.65	1.53
1	C	98	ALA	CA-CB	6.82	1.62	1.53
1	C	33	LEU	CG-CD2	6.15	1.72	1.52
1	C	105	CYS	CA-C	5.63	1.58	1.52
1	C	121	ASP	CA-C	-5.23	1.45	1.52
1	C	121	ASP	N-CA	5.17	1.52	1.46
1	C	79	GLY	C-O	-5.00	1.17	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	DC	P-O5'-C5'	-10.43	104.35	120.00
3	A	543	DA	P-O3'-C3'	7.63	131.65	120.20
2	B	505	DT	P-O3'-C3'	6.99	130.69	120.20
3	A	542	DA	P-O3'-C3'	6.71	130.26	120.20
1	C	10	PHE	N-CA-C	6.43	118.68	107.49
1	C	26	ARG	NE-CZ-NH1	6.12	127.62	121.50
1	C	121	ASP	N-CA-C	6.06	118.68	111.71
3	A	546	DC	N1-C1'-C2'	5.93	122.40	113.50
1	C	33	LEU	O-C-N	-5.87	116.46	123.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	540	DT	O4'-C1'-N1	-5.68	99.88	108.40
1	C	26	ARG	NE-CZ-NH2	-5.64	114.12	119.20
3	A	542	DA	C2'-C3'-O3'	5.45	119.68	111.50
2	B	508	DC	O3'-P-O5'	-5.38	95.93	104.00
3	A	540	DT	N1-C1'-C2'	5.37	121.55	113.50
2	B	508	DC	O4'-C1'-N1	5.33	116.39	108.40
2	B	509	DA	C2'-C3'-O3'	5.21	119.32	111.50
1	C	164	GLN	N-CA-C	5.16	119.32	112.30
2	B	502	DC	O3'-P-O5'	-5.05	96.42	104.00

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	C	1809	0	1816	44	0
2	B	264	0	147	4	1
3	A	269	0	148	1	1
4	C	12	0	6	0	0
5	A	10	0	0	0	0
5	B	6	0	0	0	0
5	C	136	0	0	11	1
All	All	2506	0	2117	48	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (48) 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:190:HIS:CD2	1:C:192:VAL:HG13	1.84	1.11
1:C:60:LYS:HG2	1:C:99:MET:HE3	1.48	0.94
1:C:190:HIS:HD2	1:C:192:VAL:HG13	1.39	0.87
1:C:214:ILE:HD11	5:C:1152:HOH:O	1.75	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LYS:CG	1:C:99:MET:HE3	2.07	0.84
1:C:214:ILE:CD1	5:C:1152:HOH:O	2.26	0.83
1:C:26:ARG:HE	1:C:81:ASN:HD21	1.29	0.80
1:C:60:LYS:HG2	1:C:99:MET:CE	2.14	0.77
1:C:178:LEU:O	1:C:209:LYS:CE	2.33	0.76
1:C:190:HIS:CD2	1:C:192:VAL:CG1	2.70	0.73
1:C:45:MET:HE1	5:C:1073:HOH:O	1.93	0.68
1:C:68:GLU:H	1:C:68:GLU:CD	2.01	0.67
1:C:190:HIS:HD2	1:C:192:VAL:H	1.44	0.66
1:C:178:LEU:O	1:C:209:LYS:HE3	1.96	0.65
1:C:60:LYS:HD3	1:C:99:MET:HE3	1.80	0.63
1:C:60:LYS:CD	1:C:99:MET:HE3	2.30	0.60
1:C:61:ILE:C	1:C:99:MET:HE2	2.30	0.57
1:C:45:MET:HE3	1:C:48:GLU:OE2	2.05	0.57
1:C:166:LYS:HD3	5:C:1089:HOH:O	2.05	0.55
1:C:35:ARG:HG3	5:C:1146:HOH:O	2.08	0.54
1:C:26:ARG:NE	1:C:81:ASN:HD21	2.02	0.53
1:C:60:LYS:HD3	1:C:99:MET:CE	2.38	0.53
1:C:214:ILE:HD12	5:C:1152:HOH:O	2.01	0.53
1:C:200:SER:O	1:C:204:GLU:HG3	2.09	0.53
1:C:87:LEU:HD13	1:C:88:TYR:CZ	2.44	0.52
1:C:26:ARG:HH21	1:C:81:ASN:ND2	2.08	0.52
2:B:510:DT:H2''	2:B:511:DG:OP2	2.11	0.50
1:C:148:ASN:HB3	2:B:502:DC:OP1	2.12	0.49
1:C:149:PRO:HB3	1:C:189:VAL:HG22	1.96	0.48
1:C:153:ILE:HD11	1:C:189:VAL:HG11	1.96	0.47
1:C:190:HIS:HD2	1:C:192:VAL:CG1	2.18	0.46
1:C:145:ASN:OD1	5:C:1143:HOH:O	2.21	0.45
1:C:114:THR:O	5:C:1088:HOH:O	2.21	0.45
1:C:87:LEU:HD13	1:C:88:TYR:CE2	2.52	0.45
1:C:110:LYS:HD2	5:C:1011:HOH:O	2.16	0.44
1:C:170:ASP:CG	5:C:1112:HOH:O	2.60	0.44
1:C:35:ARG:HD2	1:C:37:PHE:CZ	2.53	0.44
1:C:178:LEU:O	1:C:209:LYS:HE2	2.17	0.44
1:C:23:GLU:O	1:C:26:ARG:CG	2.66	0.44
1:C:64:ASP:OD2	1:C:72:GLU:OE2	2.36	0.42
1:C:26:ARG:HE	1:C:81:ASN:ND2	2.07	0.41
2:B:509:DA:C2'	2:B:510:DT:H72	2.51	0.41
1:C:45:MET:CE	5:C:1073:HOH:O	2.60	0.40
1:C:23:GLU:O	1:C:26:ARG:HG2	2.21	0.40
3:A:536:DC:H2''	3:A:537:DA:OP2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:TYR:HD1	1:C:99:MET:HE1	1.87	0.40
1:C:160:LEU:HD22	1:C:176:MET:HE1	2.03	0.40
2:B:507:DA:H2"	2:B:508:DC:OP2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:DG:P	3:A:546:DC:O3'[11_555]	1.69	0.51
5:C:1123:HOH:O	5:C:1150:HOH:O[11_555]	1.88	0.32

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	C	224/250 (90%)	213 (95%)	11 (5%)	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	C	199/220 (90%)	190 (96%)	9 (4%)	24	12

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	9	ASP
1	C	35	ARG
1	C	68	GLU
1	C	87	LEU
1	C	110	LYS
1	C	143	GLU
1	C	170	ASP
1	C	192	VAL
1	C	202	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	81	ASN
1	C	180	GLN
1	C	190	HIS
1	C	191	HIS
1	C	212	ASN
1	C	228	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](#)

1 ligand is 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
4	3C4	C	604	-	12,12,12	4.41	5 (41%)	16,16,16	2.81	8 (50%)

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
4	3C4	C	604	-	-	2/4/4/4	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	604	3C4	CZ-CE1	8.83	1.48	1.39
4	C	604	3C4	CE2-CD2	-8.54	1.25	1.38
4	C	604	3C4	CE2-CZ	5.60	1.49	1.39
4	C	604	3C4	CD1-CE1	-5.59	1.29	1.38
4	C	604	3C4	CG-CA	-2.93	1.46	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	604	3C4	CE2-CZ-CE1	-8.10	110.87	118.49
4	C	604	3C4	CE1-CD1-CA	3.26	122.57	120.46
4	C	604	3C4	CD2-CE2-CZ	3.06	123.56	120.50
4	C	604	3C4	CD1-CE1-CL	2.49	122.53	118.45
4	C	604	3C4	OH-CZ-CE2	2.42	125.86	119.36
4	C	604	3C4	CZ-CE1-CL	-2.38	115.20	119.43
4	C	604	3C4	CD1-CE1-CZ	2.19	122.20	120.92
4	C	604	3C4	O1-C-CG	2.10	121.99	113.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	604	3C4	O1-C-CG-CA
4	C	604	3C4	O2-C-CG-CA

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 ⓘ

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	C	225/250 (90%)	2.22	130 (57%) 0 0	31, 51, 60, 70	1 (0%)
2	B	13/13 (100%)	2.62	11 (84%) 0 0	54, 83, 106, 117	0
3	A	13/13 (100%)	2.76	10 (76%) 0 0	59, 78, 127, 134	0
All	All	251/276 (90%)	2.27	151 (60%) 0 0	31, 51, 83, 134	1 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	146	THR	5.5
1	C	145	ASN	5.2
1	C	141	VAL	4.8
1	C	170	ASP	4.5
1	C	188	GLY	4.4
1	C	10	PHE	4.3
1	C	232	TYR	4.3
1	C	160	LEU	4.0
1	C	171	THR	3.9
1	C	147	TYR	3.8
1	C	162	SER	3.8
1	C	228	GLN	3.8
2	B	508	DC	3.8
1	C	189	VAL	3.8
1	C	9	ASP	3.7
1	C	184	GLY	3.7
3	A	545	DG	3.7
1	C	176	MET	3.7
1	C	205	ASN	3.6
1	C	186	ILE	3.6
1	C	192	VAL	3.6
1	C	163	SER	3.6
3	A	542	DA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	198	LEU	3.6
1	C	45	MET	3.6
1	C	220	GLY	3.5
3	A	534	DG	3.4
1	C	179	SER	3.4
1	C	156	LEU	3.4
1	C	40	GLY	3.4
3	A	535	DG	3.3
2	B	509	DA	3.3
3	A	543	DA	3.3
1	C	116	PHE	3.3
1	C	187	THR	3.3
1	C	151	ILE	3.2
1	C	87	LEU	3.2
1	C	134	VAL	3.2
1	C	44	ILE	3.1
1	C	149	PRO	3.1
1	C	178	LEU	3.1
1	C	152	ARG	3.1
2	B	513	DC	3.1
1	C	229	THR	3.1
1	C	142	ALA	3.1
1	C	199	ALA	3.1
1	C	127	PHE	3.1
1	C	233	SER	3.1
1	C	32	GLY	3.1
1	C	138	ALA	3.1
1	C	165	GLY	3.1
1	C	172	TYR	3.0
2	B	506	DA	3.0
1	C	110	LYS	3.0
1	C	183	ILE	3.0
1	C	25	LEU	3.0
1	C	27	ASN	3.0
3	A	536	DC	3.0
1	C	158	TYR	2.9
1	C	150	THR	2.9
1	C	33	LEU	2.9
1	C	132	THR	2.9
1	C	208	ASP	2.9
3	A	544	DT	2.9
1	C	175	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	511	DG	2.8
1	C	111	SER	2.8
1	C	148	ASN	2.8
1	C	91	GLY	2.8
1	C	154	LEU	2.8
1	C	137	TYR	2.7
1	C	155	ARG	2.7
1	C	107	PHE	2.7
1	C	126	ILE	2.7
1	C	41	SER	2.7
1	C	217	TYR	2.7
1	C	161	CYS	2.7
2	B	510	DT	2.7
1	C	131	LEU	2.7
1	C	66	ILE	2.7
1	C	190	HIS	2.7
2	B	512	DC	2.6
1	C	180	GLN	2.6
3	A	537	DA	2.6
1	C	112	LEU	2.6
1	C	177	PRO	2.6
1	C	182[A]	SER	2.6
1	C	11	CYS	2.5
1	C	122	MET	2.5
2	B	507	DA	2.5
1	C	14	ILE	2.5
1	C	123	ILE	2.5
1	C	207	LEU	2.5
1	C	225	LEU	2.5
1	C	114	THR	2.5
3	A	546	DC	2.5
1	C	52	SER	2.5
1	C	230	SER	2.5
1	C	159	GLU	2.5
1	C	202	LYS	2.5
2	B	505	DT	2.5
1	C	136	TYR	2.4
1	C	95	TYR	2.4
1	C	144	MET	2.4
1	C	121	ASP	2.3
1	C	139	ARG	2.3
1	C	221	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	20	PHE	2.3
1	C	224	HIS	2.3
1	C	71	SER	2.3
2	B	502	DC	2.3
1	C	55	PHE	2.3
1	C	130	TYR	2.3
1	C	135	ALA	2.3
1	C	51	THR	2.3
1	C	56	LEU	2.3
1	C	118	THR	2.3
1	C	68	GLU	2.2
1	C	124	PHE	2.2
1	C	174	ILE	2.2
1	C	99	MET	2.2
1	C	223	LYS	2.2
1	C	117	ARG	2.2
3	A	541	DT	2.2
1	C	101	PRO	2.2
1	C	88	TYR	2.2
1	C	191	HIS	2.2
1	C	181	LYS	2.2
1	C	213	LYS	2.2
1	C	157	PHE	2.1
1	C	222	LEU	2.1
1	C	76	TYR	2.1
1	C	104	THR	2.1
1	C	12	GLY	2.1
1	C	35	ARG	2.1
1	C	113	ARG	2.1
1	C	214	ILE	2.1
2	B	503	DA	2.1
1	C	47	GLY	2.1
1	C	216	VAL	2.1
1	C	185	GLU	2.0
1	C	28	TYR	2.0
1	C	231	TYR	2.0
1	C	219	LEU	2.0
1	C	143	GLU	2.0
1	C	215	ILE	2.0
1	C	90	THR	2.0
1	C	18	ASN	2.0
1	C	26	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	115	VAL	2.0
1	C	168	VAL	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($\text{\AA}^2$)	Q<0.9
4	3C4	C	604	12/12	0.96	0.10	18,23,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.