



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2024 – 06:08 pm BST

PDB ID : 5L6K
Title : Crystal Structure of Human Carbonic Anhydrase II in Complex with a Quinoline Oligoamide Foldamer
Authors : Jewginski, M.; Langlois d'Estaintot, B.; Granier, T.; Huc, Y.
Deposited on : 2016-05-30
Resolution : 1.70 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

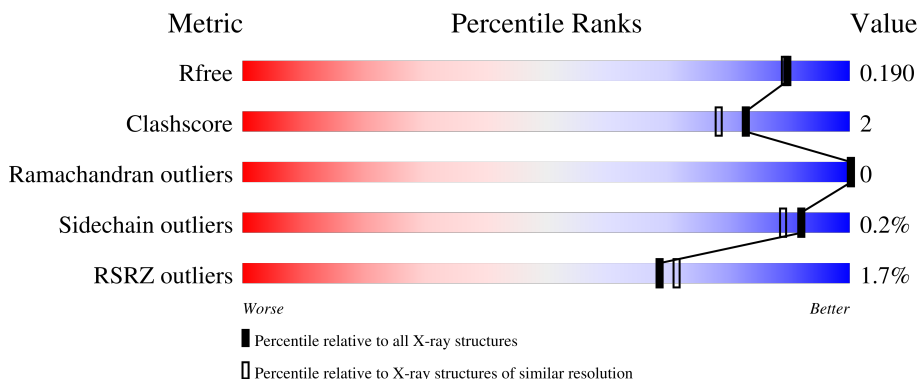
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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	260	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 95%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> </div> <p style="text-align: center;">95%</p>
1	B	260	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 96%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> </div> <p style="text-align: center;">96%</p>
2	C	6	<div style="display: flex; align-items: center;"> <div style="width: 17%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> </div> <p style="text-align: center;">17% 67% 17%</p>
2	D	6	<div style="display: flex; align-items: center;"> <div style="width: 17%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> </div> <p style="text-align: center;">17% 50% 33%</p>
3	E	5	<div style="display: flex; align-items: center;"> <div style="width: 40%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: red; margin-right: 5px;"></div> </div> <p style="text-align: center;">40% 20% 40%</p>

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Mol	Chain	Length	Quality of chain
3	F	5	 60% 40%

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 4929 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 Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	259	Total 2094	C 1351	N 358	O 383	S 2	0	8	0
1	B	259	Total 2081	C 1342	N 355	O 382	S 2	0	6	0

- Molecule 2 is a protein called Aromatic foldamer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	6	Total 95	C 67	N 11	O 16	S 1	0	0	0
2	D	6	Total 95	C 67	N 11	O 16	S 1	0	0	0

- Molecule 3 is a protein called Aromatic foldamer.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	5	Total 72	C 50	N 8	O 14	0	5	0
3	F	5	Total 64	C 46	N 8	O 10	0	5	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Zn 1	0	0
4	B	1	Total 1	Zn 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
7	A	1	4	2	1	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	220	Total	O	0	0
			220	220		
8	B	162	Total	O	0	0
			162	162		
8	C	5	Total	O	0	0
			5	5		
8	D	5	Total	O	0	0
			5	5		
8	E	4	Total	O	0	0
			4	4		
8	F	1	Total	O	0	0
			1	1		

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.

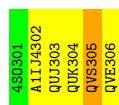
- Molecule 1: Carbonic anhydrase 2



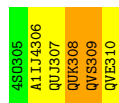
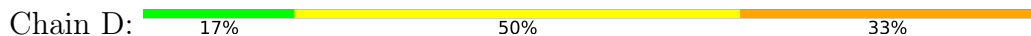
- Molecule 1: Carbonic anhydrase 2



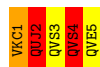
- Molecule 2: Aromatic foldamer



- Molecule 2: Aromatic foldamer



- Molecule 3: Aromatic foldamer



- Molecule 3: Aromatic foldamer

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.07Å 84.87Å 77.22Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	76.50 – 1.70 76.50 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (76.50-1.70) 99.7 (76.50-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.154 , 0.181 0.162 , 0.190	Depositor DCC
R_{free} test set	3137 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4929	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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: DMS, QVS, NA, VKC, QUJ, GOL, 4SO, ZN, QVE, QUK, A1IJ4

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	2/2178 (0.1%)	0.96	3/2956 (0.1%)
1	B	0.82	1/2162 (0.0%)	0.91	0/2934
All	All	0.86	3/4340 (0.1%)	0.94	3/5890 (0.1%)

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
2	C	0	1
2	D	0	2
3	E	0	3
3	F	0	3
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	SER	CA-CB	5.89	1.61	1.52
1	A	219	SER	CB-OG	-5.06	1.35	1.42
1	A	51	TYR	CG-CD1	5.00	1.45	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	51	TYR	CB-CG-CD1	5.19	124.11	121.00
1	A	138	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	305	QVS	Peptide
2	D	308	QUK	Peptide
2	D	309	QVS	Peptide
3	E	1[A]	VKC	Peptide
3	E	2[A]	QUJ	Peptide
3	E	4[A]	QVS	Peptide
3	F	1[B]	VKC	Peptide
3	F	2[B]	QUJ	Peptide
3	F	4[B]	QVS	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2094	0	2043	7	0
1	B	2081	0	2042	4	1
2	C	95	0	5	0	0
2	D	95	0	5	0	0
3	E	72	0	7	3	0
3	F	64	0	0	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	16	0	0
5	B	12	0	16	0	0
6	A	1	0	0	0	0
7	A	4	0	6	0	0
8	A	220	0	0	5	0
8	B	162	0	0	1	0
8	C	5	0	0	0	0
8	D	5	0	0	0	0
8	E	4	0	0	1	0
8	F	1	0	0	0	0
All	All	4929	0	4140	20	1

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 2.

All (20) 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)
3:F:1[B]:VKC:CA	3:F:4[B]:QVS:C3	2.60	0.80
3:F:1[B]:VKC:CA	3:F:4[B]:QVS:C2	2.65	0.75
1:A:17[A]:HIS:HE1	8:A:408:HOH:O	1.74	0.71
1:A:45:LYS:NZ	8:A:403:HOH:O	2.29	0.66
1:A:135:GLN:NE2	8:A:404:HOH:O	2.32	0.62
3:E:1[A]:VKC:HA	3:E:4[A]:QVS:C3	2.31	0.59
8:E:102:HOH:O	3:F:1[B]:VKC:CA	2.50	0.57
1:B:251:LYS:NZ	8:B:401:HOH:O	2.42	0.53
3:E:1[A]:VKC:HA	3:E:4[A]:QVS:C2	2.42	0.49
3:F:1[B]:VKC:O	3:F:2[B]:QUJ:C3	2.62	0.47
3:E:1[A]:VKC:O	3:E:2[A]:QUJ:C3	2.58	0.46
1:A:89:ARG:O	1:A:122:HIS:HA	2.16	0.45
3:F:2[B]:QUJ:O	3:F:3[B]:QVS:C3	2.64	0.44
3:F:4[B]:QVS:O	3:F:5[B]:QVE:C3	2.65	0.43
1:A:138:ASP:HA	8:A:465:HOH:O	2.19	0.42
1:A:80:LYS:HE2	8:A:454:HOH:O	2.20	0.41
1:B:13:PRO:HA	1:B:16:TRP:CD2	2.55	0.41
1:A:239:LEU:N	1:A:239:LEU:HD22	2.36	0.41
1:B:45:LYS:O	1:B:82:GLY:HA2	2.21	0.41

All (1) 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)
1:B:32:ASP:OD2	1:B:74:GLN:NE2[1_655]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/260 (102%)	260 (98%)	5 (2%)	0	100	100
1	B	263/260 (101%)	257 (98%)	6 (2%)	0	100	100
All	All	528/520 (102%)	517 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	225/225 (100%)	224 (100%)	1 (0%)	89	85
1	B	227/225 (101%)	227 (100%)	0	100	100
All	All	452/450 (100%)	451 (100%)	1 (0%)	92	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

18 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1IJ4	D	306	2	16,16,17	0.74	1 (6%)	17,18,20	1.01	1 (5%)
2	A1IJ4	C	302	2	16,16,17	0.96	1 (6%)	17,18,20	0.86	0
2	QUK	D	308	2	18,18,20	1.64	1 (5%)	21,24,27	2.61	6 (28%)
3	QUJ	F	2[B]	3	19,19,20	2.30	1 (5%)	23,26,28	1.76	6 (26%)
2	QVE	D	310	2	20,20,20	1.96	2 (10%)	27,28,28	1.60	5 (18%)
3	QVS	F	4[B]	3	15,15,16	2.31	2 (13%)	19,21,23	1.87	4 (21%)
3	QVS	E	4[A]	3	15,15,16	2.20	1 (6%)	19,21,23	2.10	6 (31%)
3	QVE	E	5[A]	3	20,20,20	1.93	3 (15%)	27,28,28	1.49	3 (11%)
2	QVS	C	305	2	15,15,16	2.27	2 (13%)	19,21,23	2.42	5 (26%)
3	QVS	F	3[B]	3	15,15,16	2.50	1 (6%)	19,21,23	1.97	3 (15%)
3	QVS	E	3[A]	3	15,15,16	2.14	2 (13%)	19,21,23	2.18	4 (21%)
3	QVE	F	5[B]	3	16,16,20	2.21	2 (12%)	22,23,28	1.38	2 (9%)
2	QUJ	C	303	2	18,18,20	2.00	2 (11%)	21,24,28	2.77	6 (28%)
2	QUJ	D	307	2	18,18,20	1.96	2 (11%)	21,24,28	2.35	4 (19%)
2	QVE	C	306	2	20,20,20	1.75	2 (10%)	27,28,28	1.87	5 (18%)
3	QUJ	E	2[A]	3	19,19,20	2.15	2 (10%)	23,26,28	1.72	3 (13%)
2	QUK	C	304	2	18,18,20	1.80	2 (11%)	21,24,27	2.39	5 (23%)
2	QVS	D	309	2	15,15,16	1.89	1 (6%)	19,21,23	2.33	6 (31%)

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	A1IJ4	D	306	2	-	2/10/10/11	0/1/1/1
2	A1IJ4	C	302	2	-	1/10/10/11	0/1/1/1
2	QUK	D	308	2	-	2/6/6/9	0/2/2/2
3	QUJ	F	2[B]	3	-	4/7/7/9	0/2/2/2
2	QVE	D	310	2	-	0/9/9/9	0/2/2/2
3	QVS	F	4[B]	3	-	0/2/2/4	0/2/2/2
3	QVS	E	4[A]	3	-	0/2/2/4	0/2/2/2
3	QVE	E	5[A]	3	-	0/9/9/9	0/2/2/2
2	QVS	C	305	2	-	0/2/2/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	QVS	F	3[B]	3	-	0/2/2/4	0/2/2/2
3	QVS	E	3[A]	3	-	2/2/2/4	0/2/2/2
3	QVE	F	5[B]	3	-	0/4/4/9	0/2/2/2
2	QUJ	C	303	2	-	0/6/6/9	0/2/2/2
2	QUJ	D	307	2	-	1/6/6/9	0/2/2/2
2	QVE	C	306	2	-	5/9/9/9	0/2/2/2
3	QUJ	E	2[A]	3	-	4/7/7/9	0/2/2/2
2	QUK	C	304	2	-	3/6/6/9	0/2/2/2
2	QVS	D	309	2	-	0/2/2/4	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2[B]	QUJ	CA-C	-8.96	1.39	1.48
3	F	3[B]	QVS	CA-C	-8.64	1.39	1.48
2	C	305	QVS	CA-C	-8.17	1.40	1.48
3	E	2[A]	QUJ	CA-C	-8.12	1.40	1.48
3	F	5[B]	QVE	CA-C	-7.73	1.40	1.50
3	F	4[B]	QVS	CA-C	-7.72	1.40	1.48
3	E	4[A]	QVS	CA-C	-7.60	1.40	1.48
2	D	310	QVE	CA-C	-7.46	1.40	1.50
2	C	303	QUJ	CA-C	-7.46	1.40	1.48
2	D	307	QUJ	CA-C	-7.36	1.40	1.48
3	E	3[A]	QVS	CA-C	-7.21	1.41	1.48
3	E	5[A]	QVE	CA-C	-7.01	1.41	1.50
2	D	309	QVS	CA-C	-6.55	1.41	1.48
2	C	306	QVE	CA-C	-6.54	1.41	1.50
2	C	304	QUK	C10-C	-6.52	1.41	1.48
2	D	308	QUK	C10-C	-5.75	1.42	1.48
2	C	303	QUJ	CA-N11	2.88	1.36	1.33
2	C	304	QUK	C10-N11	2.53	1.35	1.33
2	C	302	A1IJ4	C128-C127	-2.36	1.43	1.51
3	F	5[B]	QVE	OXT-C	-2.34	1.23	1.30
2	D	310	QVE	OXT-C	-2.31	1.23	1.30
3	E	2[A]	QUJ	CA-N11	2.30	1.35	1.33
2	C	306	QVE	OXT-C	-2.28	1.23	1.30
3	E	5[A]	QVE	C2-C7	-2.26	1.38	1.42
2	D	306	A1IJ4	C128-C127	-2.24	1.43	1.51
2	D	307	QUJ	CA-N11	2.17	1.35	1.33
3	E	5[A]	QVE	OXT-C	-2.17	1.23	1.30
3	E	3[A]	QVS	CA-N11	2.16	1.35	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	305	QVS	CA-N11	2.03	1.35	1.33
3	F	4[B]	QVS	C2-C7	-2.03	1.39	1.42

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	303	QUJ	CA-N11-C7	9.21	125.10	118.11
2	D	308	QUK	C10-N11-C7	8.22	124.34	118.11
2	C	304	QUK	C10-N11-C7	7.14	123.52	118.11
2	D	307	QUJ	CA-N11-C7	6.45	123.00	118.11
2	C	306	QVE	CG-OB-C8	6.29	124.12	116.95
2	D	308	QUK	C-C10-N11	6.27	120.81	114.66
3	E	3[A]	QVS	CA-N11-C7	6.25	122.85	118.11
2	C	305	QVS	CA-N11-C7	5.89	122.58	118.11
3	F	3[B]	QVS	CA-N11-C7	5.89	122.58	118.11
3	F	4[B]	QVS	CA-N11-C7	5.65	122.40	118.11
2	D	307	QUJ	C-CA-N11	5.63	120.18	114.66
3	E	2[A]	QUJ	CA-N11-C7	5.57	122.33	118.11
3	E	4[A]	QVS	CA-N11-C7	5.52	122.29	118.11
2	C	304	QUK	C-C10-N11	5.45	120.00	114.66
2	C	303	QUJ	O-C-CA	-5.32	119.18	124.22
2	D	309	QVS	C-CA-N11	4.95	119.52	114.66
3	E	4[A]	QVS	C-CA-N11	4.86	119.43	114.66
2	C	305	QVS	O-C-CA	-4.85	119.63	124.22
2	D	309	QVS	CA-N11-C7	4.51	121.53	118.11
3	F	3[B]	QVS	C9-CA-C	4.30	124.94	121.23
2	C	305	QVS	C-CA-N11	4.25	118.83	114.66
2	C	305	QVS	C3-C2-N	4.12	128.59	120.36
3	F	5[B]	QVE	OB-C8-C6	4.11	121.45	116.31
2	D	309	QVS	C3-C2-N	4.04	128.44	120.36
2	D	307	QUJ	O-C-CA	-4.00	120.43	124.22
3	E	2[A]	QUJ	C9-CA-C	3.99	124.68	121.23
3	E	5[A]	QVE	CG-OB-C8	3.99	121.50	116.95
2	D	309	QVS	O-C-CA	-3.97	120.46	124.22
3	E	3[A]	QVS	C9-CA-C	3.96	124.65	121.23
3	E	3[A]	QVS	OB-C8-C6	3.85	121.12	116.31
2	C	303	QUJ	C-CA-N11	3.79	118.37	114.66
2	D	310	QVE	C-CA-N11	3.79	122.32	116.28
3	F	2[B]	QUJ	OB-C8-C6	3.77	125.54	115.01
3	F	4[B]	QVS	C-CA-N11	3.64	118.23	114.66
2	D	310	QVE	CG-OB-C8	3.62	121.08	116.95
2	C	304	QUK	C3-CA-N	3.52	127.40	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2[B]	QUJ	O-C-CA	-3.45	120.95	124.22
3	F	2[B]	QUJ	CA-N11-C7	3.39	120.68	118.11
2	D	310	QVE	C3-C2-N	3.29	126.94	120.36
2	D	308	QUK	O-C-C10	-3.26	121.13	124.22
2	D	308	QUK	C3-CA-N	3.24	126.83	120.36
2	C	306	QVE	C-CA-N11	3.09	121.20	116.28
2	C	306	QVE	CA-N11-C7	3.06	123.68	117.24
3	F	3[B]	QVS	OB-C8-C6	3.03	120.10	116.31
2	D	307	QUJ	C3-C2-N	2.98	126.32	120.36
3	E	4[A]	QVS	C3-C2-N	2.94	126.23	120.36
2	D	306	A1IJ4	O-C-N31	-2.87	121.99	124.89
2	C	303	QUJ	C3-C2-N	2.85	126.06	120.36
2	C	306	QVE	C3-C2-N	2.74	125.84	120.36
2	C	304	QUK	O-C-C10	-2.73	121.64	124.22
3	E	3[A]	QVS	O-C-CA	-2.66	121.70	124.22
2	D	310	QVE	C9-CA-N11	-2.58	118.21	124.50
2	C	306	QVE	C9-CA-N11	-2.57	118.24	124.50
2	C	304	QUK	CG-OB-C8	2.56	125.40	117.74
3	E	5[A]	QVE	C3-C2-N	2.55	125.47	120.36
3	E	2[A]	QUJ	O-C-CA	-2.53	121.82	124.22
2	C	303	QUJ	C6-C7-N11	-2.53	117.56	122.78
3	F	4[B]	QVS	C7-C2-N	-2.48	113.35	118.07
3	F	5[B]	QVE	C-CA-N11	2.46	120.21	116.28
3	F	4[B]	QVS	C3-C2-N	2.44	125.24	120.36
3	E	5[A]	QVE	OB-C8-C6	2.43	121.81	115.01
2	D	309	QVS	OB-C8-C6	2.40	119.31	116.31
3	E	4[A]	QVS	O-C-CA	-2.40	121.95	124.22
3	E	4[A]	QVS	OB-C8-C6	2.39	119.29	116.31
3	F	2[B]	QUJ	OB-CG-CD	2.38	119.06	108.70
2	D	310	QVE	CA-N11-C7	2.36	122.22	117.24
2	C	305	QVS	C7-C2-N	-2.28	113.72	118.07
2	D	309	QVS	C3-C2-C7	-2.26	116.51	120.06
2	C	303	QUJ	C2-C7-N11	2.18	120.79	118.64
2	D	308	QUK	C7-CA-N	-2.14	113.99	118.07
3	F	2[B]	QUJ	OB-C8-C9	-2.13	117.74	124.69
3	E	4[A]	QVS	C7-C2-N	-2.09	114.09	118.07
2	D	308	QUK	C9-C10-C	2.06	123.01	121.23
3	F	2[B]	QUJ	C2-C7-N11	-2.04	116.62	118.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	304	QUK	O-C-C10-C9
2	D	308	QUK	O-C-C10-N11
2	D	308	QUK	O-C-C10-C9
2	C	306	QVE	OE1-CD-CG-OB
3	E	2[A]	QUJ	O-C-CA-C9
3	E	2[A]	QUJ	O-C-CA-N11
3	F	2[B]	QUJ	O-C-CA-C9
3	F	2[B]	QUJ	O-C-CA-N11
3	E	3[A]	QVS	O-C-CA-C9
3	E	3[A]	QVS	O-C-CA-N11
2	C	306	QVE	OE2-CD-CG-OB
2	D	306	A1IJ4	N31-C118-C119-C120
3	F	2[B]	QUJ	CE1-CD-CG-OB
2	D	306	A1IJ4	C119-C120-C121-O71
3	F	2[B]	QUJ	CE2-CD-CG-OB
2	D	307	QUJ	CD-CG-OB-C8
2	C	306	QVE	C6-C8-OB-CG
3	E	2[A]	QUJ	CE1-CD-CG-OB
2	C	306	QVE	C9-C8-OB-CG
3	E	2[A]	QUJ	CE2-CD-CG-OB
2	C	304	QUK	CE-CD-CG-OB
2	C	302	A1IJ4	C118-C119-C120-C121
2	C	306	QVE	CD-CG-OB-C8
2	C	304	QUK	O-C-C10-N11

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2[B]	QUJ	2	0
3	F	4[B]	QVS	3	0
3	E	4[A]	QVS	2	0
3	F	3[B]	QVS	1	0
3	F	5[B]	QVE	1	0
3	E	2[A]	QUJ	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 3 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
5	GOL	B	303	-	5,5,5	0.25	0	5,5,5	0.90	0
5	GOL	A	302	-	5,5,5	0.29	0	5,5,5	0.35	0
5	GOL	B	302	-	5,5,5	0.15	0	5,5,5	0.98	0
7	DMS	A	305	-	3,3,3	0.48	0	3,3,3	0.88	0
5	GOL	A	303	-	5,5,5	0.57	0	5,5,5	0.86	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	303	-	-	0/4/4/4	-
5	GOL	B	303	-	-	0/4/4/4	-
5	GOL	A	302	-	-	0/4/4/4	-
5	GOL	B	302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	302	GOL	O1-C1-C2-O2
5	B	302	GOL	O1-C1-C2-C3

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	259/260 (99%)	-0.28	3 (1%) 76 79	12, 19, 38, 64	8 (3%)
1	B	259/260 (99%)	0.01	6 (2%) 61 64	13, 24, 43, 76	6 (2%)
2	C	0/6	-	-	-	-
2	D	0/6	-	-	-	-
3	E	0/5	-	-	-	-
3	F	0/5	-	-	-	-
All	All	518/542 (95%)	-0.14	9 (1%) 69 71	12, 22, 42, 76	14 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	GLY	3.7
1	B	236	PRO	3.3
1	B	10	HIS	3.1
1	B	36	HIS	2.8
1	A	45	LYS	2.4
1	A	14[A]	GLU	2.3
1	A	4	HIS	2.3
1	B	128	GLY	2.2
1	B	2	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	QUJ	F	2[B]	18/19	0.84	0.14	17,29,38,45	18

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	QUJ	E	2[A]	18/19	0.92	0.09	13,16,23,23	18
3	QVS	F	3[B]	14/15	0.92	0.09	22,34,43,51	14
3	QVE	F	5[B]	15/19	0.93	0.11	22,30,40,46	15
3	QVS	F	4[B]	14/15	0.94	0.10	20,36,46,48	14
3	QVE	E	5[A]	19/19	0.94	0.08	10,17,30,31	19
3	QVS	E	3[A]	14/15	0.94	0.07	12,18,22,24	14
2	QUK	C	304	17/19	0.95	0.08	20,25,42,45	0
2	QVE	C	306	19/19	0.95	0.08	22,28,62,79	0
2	QUJ	C	303	17/19	0.95	0.08	19,23,40,41	0
2	QUK	D	308	17/19	0.96	0.07	20,23,36,40	0
2	A1IJ4	C	302	16/17	0.96	0.06	15,19,25,28	0
3	QVS	E	4[A]	14/15	0.96	0.06	12,18,23,26	14
2	QVE	D	310	19/19	0.96	0.07	18,23,39,44	0
2	QUJ	D	307	17/19	0.96	0.07	16,21,37,42	0
2	A1IJ4	D	306	16/17	0.96	0.08	18,24,37,40	0
2	QVS	C	305	14/15	0.97	0.05	17,19,25,25	0
2	QVS	D	309	14/15	0.98	0.04	11,16,22,23	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
5	GOL	B	303	6/6	0.83	0.15	30,37,54,54	0
7	DMS	A	305	4/4	0.83	0.18	30,33,54,92	0
6	NA	A	304	1/1	0.89	0.14	44,44,44,44	0
5	GOL	A	303	6/6	0.92	0.11	24,30,37,50	0
5	GOL	B	302	6/6	0.93	0.09	25,30,31,42	0
5	GOL	A	302	6/6	0.96	0.06	16,17,19,21	0
4	ZN	A	301	1/1	1.00	0.01	12,12,12,12	0
4	ZN	B	301	1/1	1.00	0.01	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.