



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:30 AM UTC

PDB ID : 5LVS / pdb_00005lvs
Title : Self-assembled protein-aromatic foldamer complexes with 2:3 and 2:2:1 stoichiometries
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Deposited on : 2016-09-14
Resolution : 1.42 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

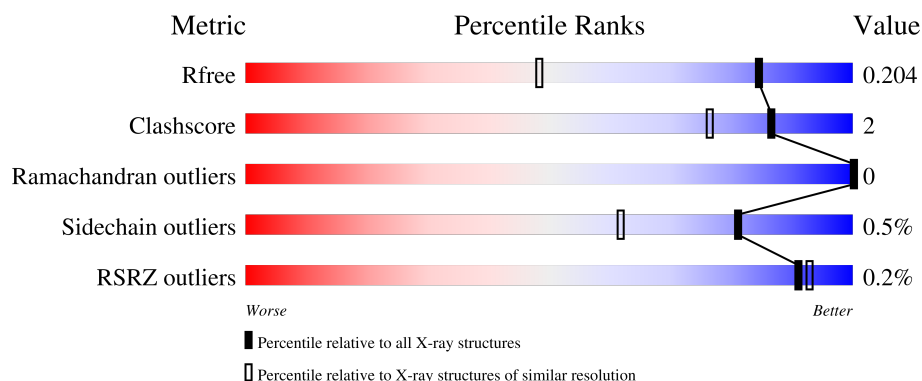
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 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	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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	259	95% 5%
1	B	259	95% 5%
2	C	6	17% 50% 33%
2	D	6	17% 17% 67%
3	H	4	100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5063 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
1	A	259	Total	C	N	O	S	0	7	0
			2070	1334	354	380	2			
1	B	259	Total	C	N	O	S	0	9	0
			2083	1342	354	385	2			

- Molecule 2 is a protein called Aromatic foldamer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	S	0	0	0
			96	68	11	16	1			
2	D	6	Total	C	N	O	S	0	0	0
			96	68	11	16	1			

- Molecule 3 is a protein called Aromatic foldamer.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	4	Total	C	N	O	0	0	0
			63	45	8	10			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	1
			12	6	6		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

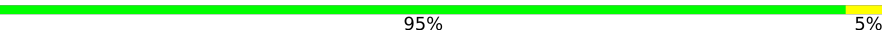
- Molecule 6 is water.

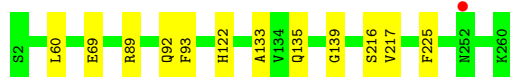
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	278	Total 278	O 278	0	0
6	B	277	Total 277	O 277	0	0
6	C	7	Total 7	O 7	0	0
6	D	7	Total 7	O 7	0	0
6	H	6	Total 6	O 6	0	0

3 Residue-property plots [i](#)

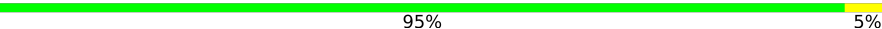
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

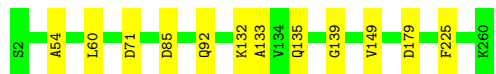
- Molecule 1: Carbonic anhydrase 2

Chain A:  95% 5%



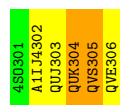
- Molecule 1: Carbonic anhydrase 2

Chain B:  95% 5%



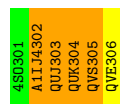
- Molecule 2: Aromatic foldamer

Chain C:  17% 50% 33%

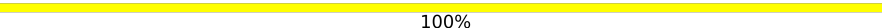


- Molecule 2: Aromatic foldamer

Chain D:  17% 17% 67%



- Molecule 3: Aromatic foldamer

Chain H:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.73Å 54.81Å 84.70Å 90.00° 112.77° 90.00°	Depositor
Resolution (Å)	45.85 – 1.42 45.85 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.85-1.42) 99.0 (45.85-1.42)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.149 , 0.178 0.186 , 0.204	Depositor DCC
R_{free} test set	6182 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5063	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4SO, A1IJ4, QVS, QUK, ZN, A1IU4, QUJ, QVE, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.88	2/2140 (0.1%)	0.91	0/2911
1	B	0.85	2/2159 (0.1%)	0.90	0/2933
All	All	0.87	4/4299 (0.1%)	0.90	0/5844

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	2
2	D	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	PHE	C-O	-6.74	1.16	1.24
1	A	225	PHE	C-O	-6.41	1.16	1.24
1	A	93	PHE	C-O	-5.41	1.17	1.23
1	B	225	PHE	CA-C	5.08	1.59	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	304	QUK	Peptide
2	C	305	QVS	Peptide

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Mol	Chain	Res	Type	Group
2	D	304	QUK	Peptide
2	D	305	QVS	Peptide

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	2070	0	1995	9	0
1	B	2083	0	2023	7	1
2	C	96	0	5	0	0
2	D	96	0	5	2	0
3	H	63	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	24	0	32	0	0
5	B	48	0	64	2	0
5	D	6	0	8	0	0
6	A	278	0	0	1	1
6	B	277	0	0	3	1
6	C	7	0	0	0	0
6	D	7	0	0	0	0
6	H	6	0	0	0	0
All	All	5063	0	4132	18	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 2.

All (18) 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)
2:D:302:A1IJ4:C	2:D:303:QUJ:N	1.68	1.50
1:A:60[B]:LEU:HD12	1:A:60[B]:LEU:O	1.94	0.68
1:B:135:GLN:NE2	6:B:401:HOH:O	2.27	0.68
1:A:216[A]:SER:O	1:A:217[A]:VAL:HG13	2.01	0.61
1:A:60[B]:LEU:HD12	1:A:60[B]:LEU:C	2.25	0.60
1:A:135:GLN:NE2	6:A:402:HOH:O	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60[B]:LEU:HD21	1:A:69:GLU:OE2	2.07	0.54
1:A:216[A]:SER:O	1:A:217[A]:VAL:CG1	2.59	0.50
2:D:302:A1IJ4:C	2:D:303:QUJ:C2	2.76	0.50
1:B:149[B]:VAL:HG12	6:B:494:HOH:O	2.11	0.49
1:B:54:ALA:HB3	5:B:307:GOL:H12	1.96	0.47
1:B:60[B]:LEU:C	1:B:60[B]:LEU:HD12	2.41	0.46
1:B:179:ASP:HA	5:B:307:GOL:H11	1.98	0.45
1:A:133:ALA:O	1:A:139:GLY:HA3	2.18	0.42
1:B:132:LYS:HG2	6:B:586:HOH:O	2.20	0.41
1:B:133:ALA:O	1:B:139:GLY:HA3	2.20	0.40
1:A:60[B]:LEU:C	1:A:60[B]:LEU:CD1	2.94	0.40
1:A:89:ARG:O	1:A:122:HIS:HA	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)
6:A:542:HOH:O	6:B:447:HOH:O[3_445]	2.17	0.03
1:B:71:ASP:OD2	1:B:85:ASP:OD2[4_454]	2.17	0.03

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	264/259 (102%)	258 (98%)	6 (2%)	0	100	100
1	B	265/259 (102%)	259 (98%)	6 (2%)	0	100	100
All	All	529/518 (102%)	517 (98%)	12 (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	218/224 (97%)	217 (100%)	1 (0%)	81	62
1	B	223/224 (100%)	222 (100%)	1 (0%)	84	67
All	All	441/448 (98%)	439 (100%)	2 (0%)	81	62

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	B	92	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	248	GLN
1	B	135	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](#)

14 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	QUJ	D	303	2	19,19,20	1.73	2 (10%)	25,26,28	2.31	4 (16%)
2	QVE	D	306	2	20,20,20	1.42	1 (5%)	28,28,28	1.66	9 (32%)
2	QVE	C	306	2	20,20,20	1.50	1 (5%)	28,28,28	1.46	6 (21%)
2	QUK	C	304	2	18,18,20	1.63	2 (11%)	23,24,27	2.46	7 (30%)
2	QUK	D	304	2	18,18,20	1.76	2 (11%)	23,24,27	2.61	8 (34%)
2	QUJ	C	303	2	19,19,20	1.59	2 (10%)	25,26,28	2.55	7 (28%)
2	A1IJ4	D	302	2	16,16,17	1.00	2 (12%)	17,18,20	1.18	1 (5%)
2	A1IJ4	C	302	2	16,16,17	1.03	1 (6%)	17,18,20	0.95	1 (5%)
2	QVS	C	305	2	15,15,16	1.75	2 (13%)	20,21,23	1.97	6 (30%)
2	QVS	D	305	2	15,15,16	1.90	2 (13%)	20,21,23	2.61	6 (30%)
3	QUK	H	303	3	15,15,20	1.53	1 (6%)	20,21,27	3.30	8 (40%)
3	QUJ	H	301	3	19,19,20	2.31	3 (15%)	25,26,28	2.95	9 (36%)
3	A1IU4	H	302	3	17,17,19	2.46	3 (17%)	21,23,27	3.96	7 (33%)
3	QUJ	H	304	3	16,16,20	1.98	4 (25%)	22,23,28	1.84	5 (22%)

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	QUJ	D	303	2	-	0/7/7/9	0/2/2/2
2	QVE	D	306	2	-	4/9/9/9	0/2/2/2
2	QVE	C	306	2	-	0/9/9/9	0/2/2/2
2	QUK	C	304	2	-	1/6/6/9	0/2/2/2
2	QUK	D	304	2	-	1/6/6/9	0/2/2/2
2	QUJ	C	303	2	-	0/7/7/9	0/2/2/2
2	A1IJ4	D	302	2	-	0/10/10/11	0/1/1/1
2	A1IJ4	C	302	2	-	0/10/10/11	0/1/1/1
2	QVS	C	305	2	-	0/2/2/4	0/2/2/2
2	QVS	D	305	2	-	0/2/2/4	0/2/2/2
3	QUK	H	303	3	-	0/2/2/9	0/2/2/2
3	QUJ	H	301	3	-	3/7/7/9	0/2/2/2
3	A1IU4	H	302	3	-	1/5/15/18	0/2/2/2
3	QUJ	H	304	3	-	0/4/4/9	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	QUJ	CA-C	-8.80	1.39	1.48
3	H	302	A1IU4	CA-N	-7.63	1.35	1.41
2	D	304	QUK	C10-C	-6.32	1.41	1.48
3	H	304	QUJ	CA-C	-6.26	1.39	1.50
2	D	303	QUJ	CA-C	-6.19	1.42	1.48
2	C	303	QUJ	CA-C	-5.86	1.42	1.48
2	C	304	QUK	C10-C	-5.73	1.42	1.48
2	D	305	QVS	CA-C	-5.68	1.42	1.48
2	D	306	QVE	CA-C	-5.25	1.41	1.50
2	C	306	QVE	CA-C	-5.21	1.41	1.50
2	C	305	QVS	CA-C	-5.06	1.43	1.48
3	H	302	A1IU4	C10-C1	-4.74	1.43	1.48
3	H	303	QUK	C10-C	-4.36	1.44	1.48
2	D	305	QVS	CA-N11	4.03	1.37	1.33
2	C	305	QVS	CA-N11	3.92	1.37	1.33
2	D	303	QUJ	C2-C7	-2.76	1.38	1.42
3	H	302	A1IU4	C4-C5	2.66	1.42	1.36
2	D	304	QUK	C10-N11	2.59	1.35	1.33
2	C	304	QUK	C10-N11	2.57	1.35	1.33
2	C	302	A1IJ4	C128-C127	-2.52	1.42	1.51
2	D	302	A1IJ4	C124-C122	2.44	1.43	1.39
3	H	301	QUJ	C2-C7	-2.38	1.38	1.42
2	C	303	QUJ	CA-N11	2.34	1.35	1.33
3	H	304	QUJ	C4-C3	2.34	1.42	1.38
3	H	304	QUJ	C2-C7	-2.30	1.38	1.42
3	H	304	QUJ	C3-C2	2.19	1.43	1.38
3	H	301	QUJ	C5-C6	-2.18	1.37	1.42
2	D	302	A1IJ4	C128-C127	-2.15	1.43	1.51

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	302	A1IU4	C1-C10-N11	12.25	126.67	114.66
3	H	301	QUJ	C-CA-N11	9.02	123.50	114.66
2	D	304	QUK	C10-N11-C7	8.05	124.69	118.06
3	H	303	QUK	C-C10-N11	7.88	122.38	114.66
3	H	302	A1IU4	C10-N11-C7	7.73	124.42	118.06
3	H	303	QUK	C10-N11-C7	7.62	124.33	118.06
2	C	303	QUJ	CA-N11-C7	7.24	124.02	118.06
2	C	304	QUK	C10-N11-C7	6.94	123.78	118.06
2	D	305	QVS	CA-N11-C7	6.82	123.67	118.06
3	H	301	QUJ	O-C-CA	-6.61	118.12	124.22
3	H	302	A1IU4	C9-C10-N11	-6.51	115.69	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	303	QUK	C9-C10-N11	-6.43	115.77	123.18
2	D	303	QUJ	CA-N11-C7	6.26	123.22	118.06
2	C	303	QUJ	C-CA-N11	6.21	120.74	114.66
3	H	302	A1IU4	C3-CA-N	6.16	131.33	123.01
2	D	303	QUJ	C9-CA-N11	-5.64	116.69	123.18
2	D	303	QUJ	C-CA-N11	5.49	120.04	114.66
2	C	303	QUJ	C9-CA-N11	-5.09	117.32	123.18
2	C	304	QUK	C9-C10-N11	-4.81	117.64	123.18
2	C	304	QUK	C-C10-N11	4.81	119.37	114.66
3	H	301	QUJ	CA-N11-C7	4.80	122.01	118.06
2	D	304	QUK	C-C10-N11	4.77	119.34	114.66
2	D	305	QVS	C-CA-N11	4.60	119.17	114.66
3	H	304	QUJ	C3-C2-N	4.48	129.28	120.39
2	C	305	QVS	CA-N11-C7	4.31	121.61	118.06
2	D	304	QUK	C9-C10-N11	-4.27	118.26	123.18
2	D	305	QVS	O-C-CA	-4.12	120.42	124.22
2	D	302	A1IJ4	O-C-N31	4.10	130.01	125.03
2	C	304	QUK	O-C-C10	-4.09	120.44	124.22
2	D	303	QUJ	O-C-CA	-4.01	120.52	124.22
2	D	305	QVS	C9-CA-N11	-4.01	118.56	123.18
3	H	301	QUJ	C3-C2-N	3.97	128.27	120.39
3	H	303	QUK	C3-CA-N	3.96	128.26	120.39
2	D	305	QVS	C3-C2-N	3.73	127.79	120.39
2	C	305	QVS	C-CA-N11	3.71	118.30	114.66
2	D	304	QUK	O-C-C10	-3.67	120.84	124.22
2	C	303	QUJ	O-C-CA	-3.63	120.87	124.22
3	H	302	A1IU4	CA-N-C	3.58	134.00	126.81
2	C	305	QVS	C3-C2-N	3.49	127.31	120.39
3	H	303	QUK	OB-C8-C6	3.41	122.27	116.42
3	H	304	QUJ	C7-C2-N	-3.31	112.03	118.16
2	C	305	QVS	O-C-CA	-3.21	121.26	124.22
3	H	301	QUJ	C9-CA-N11	-3.20	119.50	123.18
3	H	301	QUJ	C7-C2-N	-3.20	112.22	118.16
2	C	303	QUJ	C3-C2-N	3.14	126.62	120.39
3	H	303	QUK	C7-CA-N	-3.14	112.34	118.16
3	H	302	A1IU4	OB-C8-C6	3.08	121.69	116.42
2	D	306	QVE	CA-N11-C7	3.05	123.87	117.41
3	H	304	QUJ	OXT-C-CA	3.02	121.88	114.71
2	D	306	QVE	CG-OB-C8	2.96	122.99	116.68
2	D	304	QUK	CA-C7-C6	2.95	121.76	119.02
2	D	304	QUK	CG-OB-C8	2.86	126.16	117.74
2	C	306	QVE	C2-C7-C6	2.83	121.65	119.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	303	QUK	O-C-C10	-2.75	121.68	124.22
2	C	306	QVE	CG-OB-C8	2.69	122.40	116.68
2	D	306	QVE	C3-C2-N	2.68	125.70	120.39
3	H	301	QUJ	C2-C7-N11	2.64	121.33	118.55
2	C	304	QUK	C3-CA-N	2.59	125.52	120.39
2	D	306	QVE	OXT-C-O	-2.58	117.81	123.35
2	D	304	QUK	C3-CA-N	2.57	125.49	120.39
2	C	306	QVE	C3-C2-N	2.53	125.41	120.39
2	D	306	QVE	C9-CA-N11	-2.48	118.16	124.31
2	C	302	A1IJ4	O-C-N31	-2.45	122.06	125.03
2	C	303	QUJ	C2-C7-C6	2.44	121.28	119.02
3	H	301	QUJ	CG-OB-C8	2.43	126.02	118.17
2	C	305	QVS	C9-CA-N11	-2.39	120.43	123.18
2	C	304	QUK	CG-OB-C8	2.37	124.72	117.74
2	D	305	QVS	C2-C7-C6	2.36	121.21	119.02
3	H	304	QUJ	C-CA-N11	2.35	121.47	116.82
2	C	306	QVE	OXT-C-CA	2.31	120.19	114.71
3	H	301	QUJ	C9-CA-C	-2.29	117.00	121.11
2	C	303	QUJ	CG-OB-C8	2.29	125.57	118.17
2	C	306	QVE	CA-N11-C7	2.24	122.17	117.41
2	D	306	QVE	OXT-C-CA	2.20	119.94	114.71
2	C	305	QVS	C7-C2-N	-2.16	114.15	118.16
2	C	304	QUK	CA-C7-C6	2.15	121.02	119.02
2	D	306	QVE	C2-C7-C6	2.14	121.01	119.02
3	H	302	A1IU4	O-C-N	2.09	128.59	125.72
2	D	306	QVE	C6-C7-N11	-2.08	118.42	122.66
3	H	303	QUK	CA-C7-C6	2.08	120.95	119.02
2	D	306	QVE	OB-C8-C6	2.08	120.87	115.11
2	C	306	QVE	OXT-C-O	-2.07	118.90	123.35
2	D	304	QUK	C6-C7-N11	-2.00	118.57	122.66
3	H	304	QUJ	OXT-C-O	-2.00	119.05	123.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	304	QUK	O-C-C10-C9
2	D	306	QVE	C6-C8-OB-CG
2	D	306	QVE	C9-C8-OB-CG
2	D	306	QVE	OE1-CD-CG-OB
2	D	306	QVE	OE2-CD-CG-OB
3	H	302	A1IU4	O-C-N-CA

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Mol	Chain	Res	Type	Atoms
3	H	301	QUJ	CE1-CD-CG-OB
3	H	301	QUJ	CD-CG-OB-C8
3	H	301	QUJ	CE2-CD-CG-OB
2	C	304	QUK	O-C-C10-C9

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	303	QUJ	2	0
2	D	302	A1IJ4	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	A	304	-	5,5,5	0.45	0	5,5,5	0.38	0
5	GOL	B	305	-	5,5,5	0.66	0	5,5,5	0.56	0
5	GOL	B	303[B]	-	5,5,5	0.40	0	5,5,5	0.66	0
5	GOL	A	302	-	5,5,5	0.43	0	5,5,5	0.95	0
5	GOL	B	303[A]	-	5,5,5	0.65	0	5,5,5	0.87	0
5	GOL	B	308	-	5,5,5	0.29	0	5,5,5	0.48	0
5	GOL	D	401	-	5,5,5	0.22	0	5,5,5	0.72	0
5	GOL	B	307	-	5,5,5	0.40	0	5,5,5	0.52	0
5	GOL	B	302	-	5,5,5	0.52	0	5,5,5	0.45	0
5	GOL	B	306	-	5,5,5	0.31	0	5,5,5	0.89	0
5	GOL	A	303	-	5,5,5	0.55	0	5,5,5	0.62	0
5	GOL	A	305	-	5,5,5	0.15	0	5,5,5	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	304	-	5,5,5	0.38	0	5,5,5	0.45	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
5	GOL	A	304	-	-	0/4/4/4	-
5	GOL	B	305	-	-	0/4/4/4	-
5	GOL	B	303[B]	-	-	0/4/4/4	-
5	GOL	A	302	-	-	0/4/4/4	-
5	GOL	B	303[A]	-	-	0/4/4/4	-
5	GOL	B	308	-	-	0/4/4/4	-
5	GOL	D	401	-	-	0/4/4/4	-
5	GOL	B	307	-	-	4/4/4/4	-
5	GOL	B	302	-	-	0/4/4/4	-
5	GOL	B	306	-	-	2/4/4/4	-
5	GOL	A	303	-	-	0/4/4/4	-
5	GOL	A	305	-	-	0/4/4/4	-
5	GOL	B	304	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	307	GOL	O1-C1-C2-O2
5	B	307	GOL	O1-C1-C2-C3
5	B	306	GOL	O1-C1-C2-C3
5	B	307	GOL	C1-C2-C3-O3
5	B	307	GOL	O2-C2-C3-O3
5	B	306	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	307	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	2
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	303:QUK	C	304:QUJ	N	3.88
1	H	301:QUJ	C	302:A1IU4	N	3.67
1	D	302:A1IJ4	C	303:QUJ	N	1.68

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	259/259 (100%)	-0.20	1 (0%) 88 91	11, 26, 42, 55	7 (2%)
1	B	259/259 (100%)	-0.21	0 100 100	11, 25, 40, 57	8 (3%)
2	C	0/6	-	-	-	-
2	D	0/6	-	-	-	-
3	H	0/4	-	-	-	-
All	All	518/534 (97%)	-0.21	1 (0%) 91 93	11, 25, 41, 57	15 (2%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	ASN	2.6

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	H	301	18/19	0.91	0.11	21,30,37,38	0
3	A1IU4	H	302	16/18	0.94	0.09	24,33,44,45	0
3	QUK	H	303	14/19	0.94	0.09	24,31,39,39	0
3	QUJ	H	304	15/19	0.95	0.07	24,29,41,42	0
2	QVE	C	306	19/19	0.96	0.08	26,32,56,62	0
2	A1IJ4	D	302	16/17	0.97	0.06	23,26,29,30	0
2	QUK	D	304	17/19	0.97	0.08	27,31,41,42	0
2	A1IJ4	C	302	16/17	0.97	0.06	21,24,26,26	0
2	QVE	D	306	19/19	0.97	0.07	27,31,63,65	0
2	QUJ	C	303	18/19	0.98	0.06	24,25,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	QVS	D	305	14/15	0.98	0.05	23,24,27,32	0
2	QUJ	D	303	18/19	0.98	0.06	25,28,36,39	0
2	QUK	C	304	17/19	0.98	0.06	24,29,39,47	0
2	QVS	C	305	14/15	0.99	0.04	22,23,26,30	0

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
5	GOL	B	302	6/6	0.85	0.13	37,38,43,46	0
5	GOL	B	307	6/6	0.88	0.13	38,39,41,45	0
5	GOL	A	302	6/6	0.89	0.12	31,33,37,41	0
5	GOL	B	305	6/6	0.89	0.13	36,40,45,48	0
5	GOL	A	305	6/6	0.89	0.11	31,33,40,44	0
5	GOL	B	308	6/6	0.90	0.10	31,34,39,47	0
5	GOL	B	303[B]	6/6	0.91	0.10	11,12,17,19	6
5	GOL	B	303[A]	6/6	0.91	0.10	17,19,20,25	6
5	GOL	B	306	6/6	0.93	0.10	25,29,31,41	1
5	GOL	D	401	6/6	0.93	0.10	27,35,42,48	0
5	GOL	B	304	6/6	0.94	0.09	27,29,31,36	0
5	GOL	A	303	6/6	0.96	0.11	18,20,22,25	0
5	GOL	A	304	6/6	0.96	0.08	28,29,30,35	0
4	ZN	A	301	1/1	0.99	0.03	18,18,18,18	0
4	ZN	B	301	1/1	1.00	0.02	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.