wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2024 – 07:29 pm BST

PDB ID	:	5LVS
Title	:	Self-assembled protein-aromatic foldamer complexes with 2:3 and 2:2:1 stoichiometries
Authors	:	Jewginski, M.; LANGLOIS D'ESTAINTOT, B.; Granier, T.; Huc, Y.
Deposited on	:	2016-09-14
Resolution	:	1.42 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

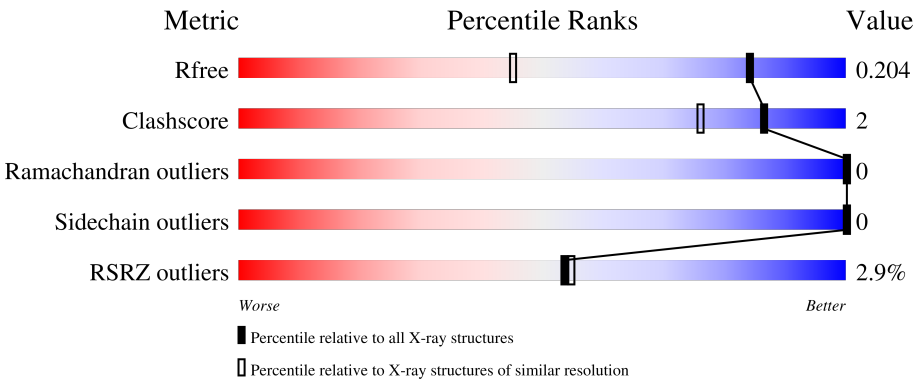
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.42 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}	164625	3500 (1.44-1.40)
Clashscore	180529	3801 (1.44-1.40)
Ramachandran outliers	177936	3734 (1.44-1.40)
Sidechain outliers	177891	3733 (1.44-1.40)
RSRZ outliers	164620	3499 (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 <=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	3%, 95%, 5%
1	B	259	3%, 96%, .
2	C	6	17%, 50%, 33%
2	D	6	17%, 17%, 67%
3	E	5	20%, 60%, 20%

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
			Total	C	N	O	S			
1	A	259	2070	1334	354	380	2	0	7	0
1	B	259	2083	1342	354	385	2	0	9	0

- Molecule 2 is a protein called Aromatic foldamer.

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

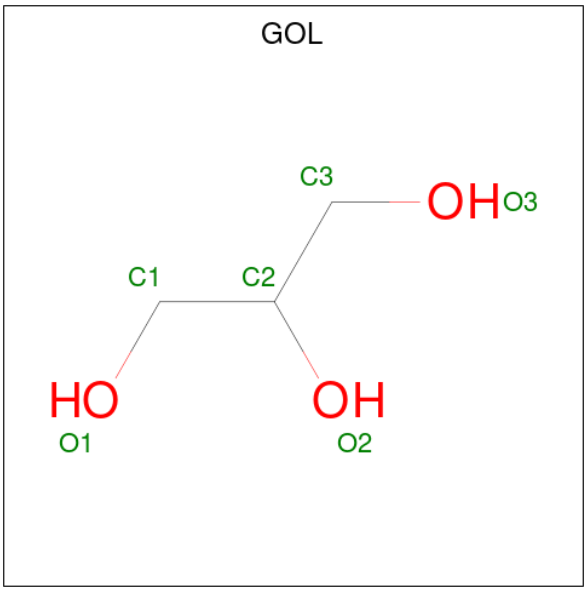
- Molecule 3 is a protein called Aromatic foldamer.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	5	63	45	8	10	0	0	1

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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

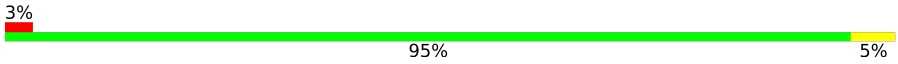
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	278	278	278	0	0
			Total	O		
6	B	277	277	277	0	0
			Total	O		
6	C	7	7	7	0	0
			Total	O		
6	D	7	7	7	0	0
			Total	O		
6	E	6	6	6	0	0

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.

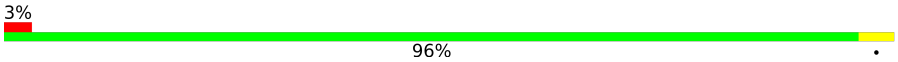
- Molecule 1: Carbonic anhydrase 2

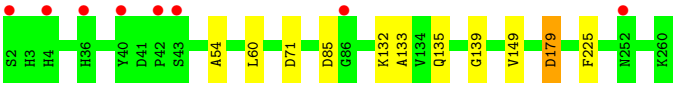
Chain A:



- Molecule 1: Carbonic anhydrase 2

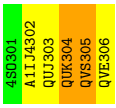
Chain B:





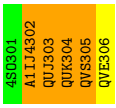
- Molecule 2: Aromatic foldamer

Chain C:



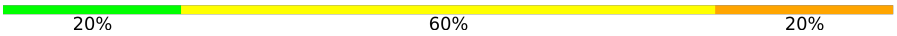
- Molecule 2: Aromatic foldamer

Chain D:



- Molecule 3: Aromatic foldamer

Chain E:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.99 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.149 , 0.178 0.184 , 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)	0.39 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]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 (i)

5.1 Standard geometry (i)

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

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	0.69	0/2140	0.86	3/2911 (0.1%)
1	B	0.68	0/2159	0.87	2/2933 (0.1%)
All	All	0.68	0/4299	0.87	5/5844 (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	2
2	D	0	2
3	E	0	1
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	225	PHE	CB-CG-CD2	-6.20	116.46	120.80
1	A	52	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	140	LEU	CB-CG-CD2	5.67	120.64	111.00
1	B	179	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	226	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	304	QUK	Peptide
2	C	305	QVS	Peptide
2	D	304	QUK	Peptide
2	D	305	QVS	Peptide
3	E	304	QUK	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	2070	0	1995	8	0
1	B	2083	0	2023	7	1
2	C	96	0	5	0	0
2	D	96	0	5	2	0
3	E	63	0	2	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	E	6	0	0	0	0
All	All	5063	0	4134	17	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.

The worst 5 of 17 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLN:NE2	6:A:402:HOH:O	2.36	0.56

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%)	218 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	223/224 (100%)	223 (100%)	0	100	100
All	All	441/448 (98%)	441 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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)

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	C	303	2	19,19,20	1.60	2 (10%)	23,26,28	2.45	5 (21%)
2	QUK	D	304	2	18,18,20	1.77	2 (11%)	21,24,27	2.58	6 (28%)
2	QUK	C	304	2	18,18,20	1.64	2 (11%)	21,24,27	2.39	5 (23%)
2	QVS	C	305	2	15,15,16	1.75	2 (13%)	19,21,23	1.99	6 (31%)
3	QUJ	E	301	3	19,19,20	2.34	3 (15%)	23,26,28	3.13	8 (34%)
3	QUK	E	302	3	15,15,20	1.51	1 (6%)	19,21,27	3.26	7 (36%)
3	QUK	E	304	3	15,15,20	1.71	2 (13%)	19,21,27	4.17	7 (36%)
2	QVE	C	306	2	20,20,20	1.78	1 (5%)	27,28,28	1.62	7 (25%)
2	A1IJ4	D	302	2	16,16,17	1.02	2 (12%)	17,18,20	1.38	1 (5%)
2	QVE	D	306	2	20,20,20	1.72	1 (5%)	27,28,28	1.89	9 (33%)
2	QUJ	D	303	2	19,19,20	1.74	2 (10%)	23,26,28	2.18	4 (17%)
2	QVS	D	305	2	15,15,16	1.89	2 (13%)	19,21,23	2.56	4 (21%)
2	A1IJ4	C	302	2	16,16,17	1.01	1 (6%)	17,18,20	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	QUJ	E	305	3	16,16,20	2.33	3 (18%)	22,23,28	1.95	6 (27%)

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

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	301	QUJ	CA-C	-9.00	1.39	1.48
3	E	305	QUJ	CA-C	-8.13	1.39	1.50
2	D	306	QVE	CA-C	-6.84	1.41	1.50
2	C	306	QVE	CA-C	-6.78	1.41	1.50
2	D	304	QUK	C10-C	-6.44	1.41	1.48

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	304	QUK	C-C10-N11	12.25	126.67	114.66
3	E	301	QUJ	C-CA-N11	9.02	123.50	114.66
2	D	304	QUK	C10-N11-C7	8.68	124.69	118.11
3	E	304	QUK	C10-N11-C7	8.32	124.42	118.11
3	E	302	QUK	C10-N11-C7	8.21	124.33	118.11

There are no chirality outliers.

5 of 8 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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	302	A1IJ4	2	0
2	D	303	QUJ	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	0.44	0	5,5,5	0.34	0
5	GOL	D	401	-	5,5,5	0.22	0	5,5,5	0.65	0
5	GOL	B	302	-	5,5,5	0.52	0	5,5,5	0.41	0
5	GOL	B	308	-	5,5,5	0.28	0	5,5,5	0.44	0
5	GOL	B	303[B]	-	5,5,5	0.39	0	5,5,5	0.62	0
5	GOL	B	305	-	5,5,5	0.64	0	5,5,5	0.53	0
5	GOL	B	307	-	5,5,5	0.38	0	5,5,5	0.48	0
5	GOL	B	303[A]	-	5,5,5	0.62	0	5,5,5	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	A	305	-	5,5,5	0.15	0	5,5,5	0.69	0
5	GOL	A	303	-	5,5,5	0.52	0	5,5,5	0.60	0
5	GOL	A	302	-	5,5,5	0.42	0	5,5,5	0.88	0
5	GOL	B	306	-	5,5,5	0.30	0	5,5,5	0.82	0
5	GOL	B	304	-	5,5,5	0.37	0	5,5,5	0.40	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	D	401	-	-	0/4/4/4	-
5	GOL	B	302	-	-	0/4/4/4	-
5	GOL	B	308	-	-	0/4/4/4	-
5	GOL	B	303[B]	-	-	1/4/4/4	-
5	GOL	B	305	-	-	0/4/4/4	-
5	GOL	B	307	-	-	4/4/4/4	-
5	GOL	B	303[A]	-	-	0/4/4/4	-
5	GOL	A	305	-	-	0/4/4/4	-
5	GOL	A	303	-	-	0/4/4/4	-
5	GOL	A	302	-	-	0/4/4/4	-
5	GOL	B	306	-	-	2/4/4/4	-
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.

5 of 7 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

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
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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%)	0.18	7 (2%) 56 57	11, 26, 42, 55	7 (2%)
1	B	259/259 (100%)	0.20	8 (3%) 51 52	11, 25, 40, 57	8 (3%)
2	C	0/6	-	-	-	-
2	D	0/6	-	-	-	-
3	E	0/5	-	-	-	-
All	All	518/535 (96%)	0.19	15 (2%) 54 55	11, 25, 41, 57	15 (2%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	ASN	3.2
1	A	40	TYR	3.0
1	A	36	HIS	2.8
1	B	2	SER	2.8
1	B	42	PRO	2.7

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	E	301	18/19	0.84	0.14	21,30,37,38	0
3	QUJ	E	305	15/19	0.87	0.11	24,29,41,42	0
3	QUK	E	302	14/19	0.88	0.13	24,31,39,39	0
3	QUK	E	304	14/19	0.89	0.12	24,33,39,42	0
2	QVE	C	306	19/19	0.92	0.10	26,32,56,62	0
2	QUK	D	304	17/19	0.93	0.11	27,31,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	QVE	D	306	19/19	0.93	0.10	27,31,63,65	0
2	QUJ	D	303	18/19	0.94	0.09	25,28,36,39	0
2	A1IJ4	D	302	16/17	0.95	0.07	23,26,29,30	0
2	QVS	D	305	14/15	0.95	0.07	23,24,27,32	0
2	A1IJ4	C	302	16/17	0.95	0.07	21,24,26,26	0
2	QUK	C	304	17/19	0.95	0.09	24,29,39,47	0
2	QUJ	C	303	18/19	0.96	0.08	24,25,40,40	0
2	QVS	C	305	14/15	0.98	0.05	22,23,26,30	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(Å^2)	Q<0.9
5	GOL	B	302	6/6	0.77	0.16	37,38,43,46	0
5	GOL	A	305	6/6	0.82	0.14	31,33,40,44	0
5	GOL	A	302	6/6	0.83	0.14	31,33,37,41	0
5	GOL	B	307	6/6	0.83	0.15	38,39,41,45	0
5	GOL	B	305	6/6	0.84	0.14	36,40,45,48	0
5	GOL	B	303[A]	6/6	0.86	0.13	17,19,20,25	6
5	GOL	B	303[B]	6/6	0.86	0.13	11,12,17,19	6
5	GOL	B	306	6/6	0.87	0.13	25,29,31,41	1
5	GOL	B	308	6/6	0.88	0.12	31,34,39,47	0
5	GOL	D	401	6/6	0.88	0.14	27,35,42,48	0
5	GOL	B	304	6/6	0.89	0.12	27,29,31,36	0
5	GOL	A	304	6/6	0.91	0.10	28,29,30,35	0
5	GOL	A	303	6/6	0.96	0.12	18,20,22,25	0
4	ZN	B	301	1/1	1.00	0.02	19,19,19,19	0
4	ZN	A	301	1/1	1.00	0.02	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.