



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:26 PM UTC

PDB ID : 8D2J / pdb_00008d2j
Title : A novel insecticidal protein from ferns IPD113_Cow.
Authors : Maher, M.J.
Deposited on : 2022-05-30
Resolution : 2.10 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

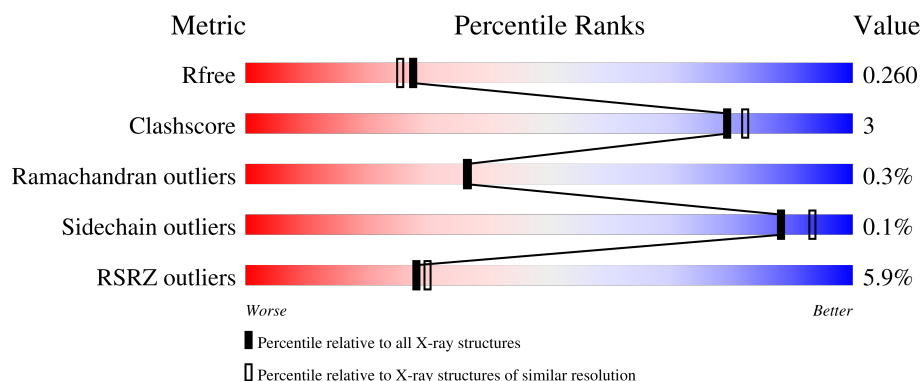
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	512	
1	B	512	
1	C	512	
1	D	512	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16286 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 IPD113_Cow.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	483	Total	C	N	O	S	0	5	0
			3919	2483	689	733	14			
1	A	479	Total	C	N	O	S	0	1	0
			3862	2447	682	719	14			
1	C	478	Total	C	N	O	S	0	1	0
			3860	2445	681	720	14			
1	D	480	Total	C	N	O	S	0	0	0
			3876	2455	683	724	14			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

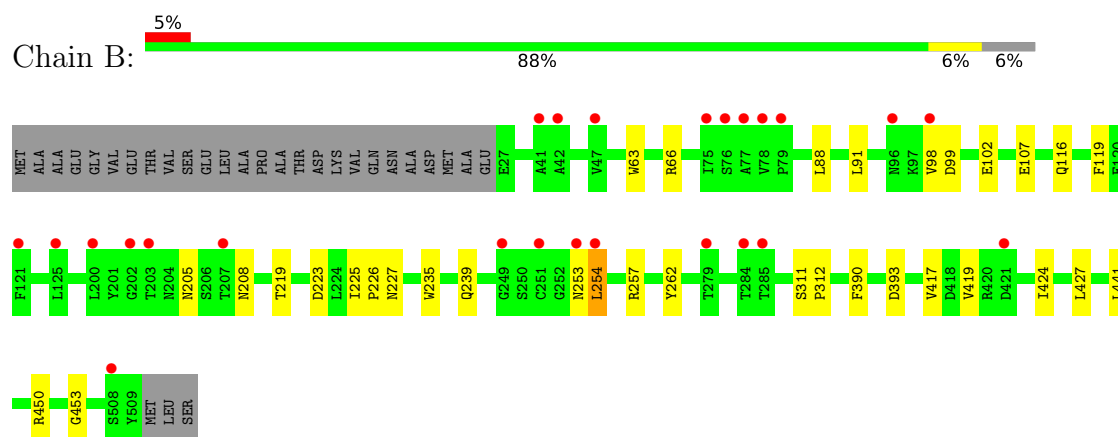
- Molecule 3 is water.

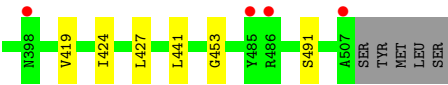
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	204	Total	O	0	0
			204	204		
3	A	221	Total	O	0	0
			221	221		
3	C	175	Total	O	0	0
			175	175		
3	D	145	Total	O	0	0
			145	145		

3 Residue-property plots [i](#)

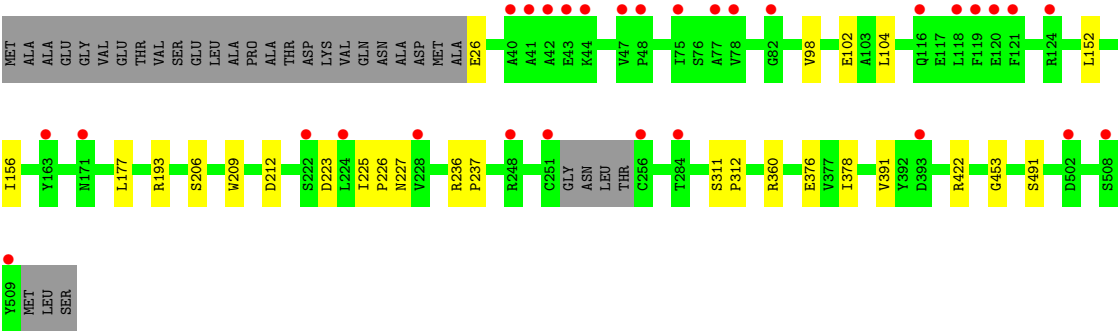
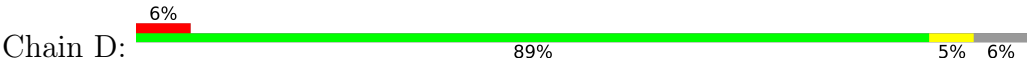
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: IPD113_Cow





● Molecule 1: IPD113_Cow



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.64Å 79.39Å 108.55Å 97.92° 104.95° 97.41°	Depositor
Resolution (Å)	47.82 – 2.10 47.82 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.82-2.10) 97.2 (47.82-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.220 , 0.256 0.224 , 0.260	Depositor DCC
R_{free} test set	6955 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16286	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: 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	0.99	0/3959	1.42	1/5381 (0.0%)
1	B	0.99	0/4030	1.43	1/5479 (0.0%)
1	C	0.99	0/3956	1.44	1/5376 (0.0%)
1	D	1.00	0/3970	1.43	1/5395 (0.0%)
All	All	0.99	0/15915	1.43	4/21631 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	GLY	CA-C-O	-5.95	118.13	122.23
1	D	453	GLY	CA-C-O	-5.77	118.25	122.23
1	B	453	GLY	CA-C-O	-5.72	118.28	122.23
1	C	453	GLY	CA-C-O	-5.20	118.08	122.29

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	A	3862	0	3754	25	0
1	B	3919	0	3815	23	0
1	C	3860	0	3752	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3876	0	3766	18	0
2	A	6	0	8	0	0
2	C	12	0	16	1	0
2	D	6	0	8	0	0
3	A	221	0	0	1	0
3	B	204	0	0	1	0
3	C	175	0	0	2	0
3	D	145	0	0	2	0
All	All	16286	0	15119	83	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (83) 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:B:253:ASN:O	1:B:254:LEU:HB3	1.85	0.77
1:C:104:LEU:O	1:C:110:ILE:HD11	1.89	0.72
1:B:98:VAL:CG1	1:B:102:GLU:HB3	2.29	0.63
1:B:107[B]:GLU:OE2	1:B:107[B]:GLU:HA	1.99	0.61
1:D:422:ARG:O	3:D:701:HOH:O	2.15	0.60
1:D:152:LEU:HD22	3:D:702:HOH:O	2.01	0.59
1:A:104:LEU:HD11	1:A:177:LEU:HB3	1.86	0.58
1:B:205:ASN:HD21	1:B:208:ASN:HD22	1.51	0.57
1:A:116:GLN:HA	1:A:119:PHE:CE2	2.39	0.57
1:A:98:VAL:HG13	1:A:102:GLU:HB3	1.87	0.55
1:A:107[B]:GLU:OE2	1:A:107[B]:GLU:HA	2.07	0.55
1:B:253:ASN:O	1:B:254:LEU:CB	2.56	0.54
1:B:390:PHE:CD2	3:B:720:HOH:O	2.54	0.54
1:C:104:LEU:HD11	1:C:177:LEU:HB3	1.88	0.54
1:D:26:GLU:OE1	1:D:26:GLU:N	2.41	0.53
1:D:152:LEU:O	1:D:156:ILE:HG12	2.08	0.53
1:C:98:VAL:HG13	1:C:102:GLU:HB3	1.91	0.53
1:C:107[B]:GLU:OE2	1:C:107[B]:GLU:HA	2.09	0.53
1:C:427:LEU:CD2	1:C:441:LEU:HD22	2.38	0.53
1:B:417:VAL:HG11	1:B:441:LEU:HD12	1.91	0.53
1:C:101:TRP:O	1:C:104:LEU:HB3	2.08	0.53
1:D:223:ASP:OD1	1:D:227:ASN:ND2	2.42	0.53
1:B:98:VAL:HG13	1:B:102:GLU:HB3	1.90	0.52
1:C:98:VAL:CG1	1:C:102:GLU:HB3	2.40	0.52
1:D:98:VAL:CG1	1:D:102:GLU:HB3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:NH2	1:A:212:ASP:OD2	2.42	0.51
1:D:225:ILE:HB	1:D:226:PRO:HD3	1.95	0.49
1:A:101:TRP:O	1:A:104:LEU:HB3	2.13	0.49
1:D:104:LEU:HD11	1:D:177:LEU:HB3	1.95	0.48
1:C:116:GLN:HA	1:C:119:PHE:CE2	2.49	0.48
1:B:257:ARG:NH1	1:A:99:ASP:OD1	2.46	0.48
1:B:311:SER:N	1:B:312:PRO:CD	2.77	0.48
1:A:365:ARG:NH1	3:A:702:HOH:O	2.46	0.48
1:C:341:ARG:NH2	3:C:701:HOH:O	2.46	0.48
1:D:311:SER:N	1:D:312:PRO:CD	2.76	0.47
1:A:426:GLU:HB2	1:A:442:HIS:HB3	1.96	0.47
1:A:219:THR:O	1:A:223:ASP:HB3	2.14	0.46
1:C:225:ILE:HB	1:C:226:PRO:HD3	1.97	0.46
1:A:378:ILE:HD12	1:A:378:ILE:N	2.31	0.46
1:C:311:SER:N	1:C:312:PRO:CD	2.78	0.46
1:A:253:ASN:O	1:A:254:LEU:CB	2.63	0.45
1:C:139:ARG:O	1:C:143:ALA:HB2	2.17	0.45
1:C:219:THR:O	1:C:223:ASP:HB3	2.17	0.45
1:A:311:SER:N	1:A:312:PRO:CD	2.80	0.45
1:A:104:LEU:HD11	1:A:177:LEU:CB	2.46	0.45
1:C:419:VAL:HG11	1:C:424:ILE:HD11	1.97	0.45
1:D:193:ARG:NH2	1:D:212:ASP:OD2	2.49	0.45
1:B:235:TRP:HZ2	1:B:239:GLN:HE21	1.64	0.44
1:A:225:ILE:HB	1:A:226:PRO:HD3	1.98	0.44
1:A:427:LEU:HD22	1:A:441:LEU:HD22	2.00	0.44
1:C:160:ASP:O	1:C:164:ILE:HG12	2.17	0.44
1:B:107[B]:GLU:OE2	1:B:107[B]:GLU:CA	2.66	0.43
1:B:262:TYR:OH	1:A:102:GLU:OE2	2.32	0.43
1:A:243:SER:O	1:A:263:ALA:HA	2.19	0.43
1:B:66:ARG:HD3	1:B:91:LEU:O	2.19	0.43
2:C:602:GOL:H12	3:C:710:HOH:O	2.17	0.43
1:B:225:ILE:HB	1:B:226:PRO:HD3	2.01	0.42
1:C:109:TYR:HB3	1:C:305:ASP:HB3	1.99	0.42
1:C:360:ARG:HD3	1:C:491:SER:HB2	2.01	0.42
1:B:223:ASP:OD1	1:B:227:ASN:ND2	2.51	0.42
1:D:378:ILE:HD12	1:D:378:ILE:N	2.35	0.42
1:B:99:ASP:OD1	1:A:257:ARG:NH1	2.53	0.42
1:A:427:LEU:CD2	1:A:441:LEU:HD22	2.49	0.42
1:D:378:ILE:HD13	1:D:391:VAL:HG23	2.02	0.42
1:B:219:THR:O	1:B:223:ASP:HB3	2.20	0.42
1:A:63:TRP:HB3	1:A:107[B]:GLU:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:VAL:CG1	1:A:102:GLU:HB3	2.50	0.42
1:B:63:TRP:HB3	1:B:107[B]:GLU:CD	2.45	0.41
1:D:104:LEU:HD11	1:D:177:LEU:CB	2.50	0.41
1:A:109:TYR:HB3	1:A:305:ASP:HB3	2.02	0.41
1:C:104:LEU:HD11	1:C:177:LEU:CB	2.50	0.41
1:A:253:ASN:O	1:A:254:LEU:HB3	2.21	0.41
1:B:88:LEU:HD23	1:B:88:LEU:C	2.46	0.41
1:D:206:SER:HA	1:D:209:TRP:CE3	2.55	0.41
1:B:116:GLN:HA	1:B:119:PHE:CE2	2.55	0.41
1:A:155:TRP:CD1	1:A:155:TRP:C	2.99	0.41
1:D:98:VAL:HG13	1:D:102:GLU:HB3	2.03	0.41
1:D:376:GLU:HB2	1:D:391:VAL:HB	2.03	0.41
1:D:236:ARG:N	1:D:237:PRO:CD	2.85	0.40
1:B:427:LEU:CD2	1:B:441:LEU:HD22	2.51	0.40
1:D:360:ARG:HD3	1:D:491:SER:HB2	2.04	0.40
1:B:419:VAL:HG11	1:B:424:ILE:HD11	2.03	0.40
1:C:115:GLN:HE21	1:C:235:TRP:HZ2	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	476/512 (93%)	463 (97%)	11 (2%)	2 (0%)	30	28
1	B	486/512 (95%)	473 (97%)	11 (2%)	2 (0%)	30	28
1	C	475/512 (93%)	465 (98%)	9 (2%)	1 (0%)	43	44
1	D	476/512 (93%)	465 (98%)	11 (2%)	0	100	100
All	All	1913/2048 (93%)	1866 (98%)	42 (2%)	5 (0%)	36	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	254	LEU
1	A	254	LEU
1	C	79	PRO
1	B	450	ARG
1	A	79	PRO

5.3.2 Protein sidechains ⓘ

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	414/440 (94%)	414 (100%)	0	100	100
1	B	423/440 (96%)	421 (100%)	2 (0%)	81	88
1	C	414/440 (94%)	414 (100%)	0	100	100
1	D	416/440 (94%)	416 (100%)	0	100	100
All	All	1667/1760 (95%)	1665 (100%)	2 (0%)	88	93

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

Mol	Chain	Res	Type
1	B	393[A]	ASP
1	B	393[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	115	GLN
1	B	150	ASN
1	B	208	ASN
1	B	358	ASN
1	A	158	GLN
1	C	115	GLN
1	C	205	ASN
1	C	280	ASN
1	D	57	GLN
1	D	128	ASN

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Mol	Chain	Res	Type
1	D	383	HIS
1	D	398	ASN
1	D	496	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](#)

4 ligands 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	GOL	C	601	-	5,5,5	0.07	0	5,5,5	0.23	0
2	GOL	D	601	-	5,5,5	0.08	0	5,5,5	0.28	0
2	GOL	A	601	-	5,5,5	0.08	0	5,5,5	0.26	0
2	GOL	C	602	-	5,5,5	0.07	0	5,5,5	0.25	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
2	GOL	C	601	-	-	0/4/4/4	-
2	GOL	D	601	-	-	0/4/4/4	-
2	GOL	A	601	-	-	2/4/4/4	-
2	GOL	C	602	-	-	0/4/4/4	-

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
2	A	601	GOL	C1-C2-C3-O3
2	A	601	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	479/512 (93%)	0.60	21 (4%)	39	41	18, 30, 45, 57	1 (0%)
1	B	483/512 (94%)	0.61	25 (5%)	33	35	16, 32, 49, 63	5 (1%)
1	C	478/512 (93%)	0.81	38 (7%)	18	20	20, 35, 54, 77	1 (0%)
1	D	480/512 (93%)	0.79	30 (6%)	26	27	26, 36, 52, 73	0
All	All	1920/2048 (93%)	0.70	114 (5%)	28	30	16, 33, 51, 77	7 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	VAL	5.3
1	C	369	THR	5.2
1	C	46	GLU	5.2
1	D	77	ALA	4.9
1	D	40	ALA	4.4
1	C	79	PRO	4.3
1	D	42	ALA	4.1
1	D	251	CYS	3.9
1	D	47	VAL	3.8
1	A	121	PHE	3.8
1	C	507	ALA	3.7
1	D	118	LEU	3.7
1	C	256	CYS	3.6
1	D	41	ALA	3.6
1	B	254	LEU	3.5
1	C	370	LEU	3.5
1	B	47	VAL	3.5
1	C	78	VAL	3.3
1	C	251	CYS	3.3
1	D	393	ASP	3.2
1	C	76	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	207	THR	3.2
1	B	77	ALA	3.1
1	A	72	LEU	3.1
1	B	253	ASN	3.0
1	B	121	PHE	3.0
1	A	40	ALA	3.0
1	D	78	VAL	3.0
1	C	202	GLY	3.0
1	A	42	ALA	3.0
1	C	203	THR	3.0
1	B	78	VAL	2.9
1	D	256	CYS	2.9
1	B	98	VAL	2.9
1	B	75	ILE	2.9
1	C	44	LYS	2.9
1	D	121	PHE	2.8
1	B	79	PRO	2.8
1	C	247	ARG	2.7
1	D	124	ARG	2.7
1	A	253	ASN	2.7
1	D	119	PHE	2.7
1	C	398	ASN	2.7
1	C	98	VAL	2.7
1	D	171	ASN	2.7
1	B	42	ALA	2.6
1	B	284	THR	2.6
1	C	384	HIS	2.6
1	C	45	GLU	2.6
1	D	224	LEU	2.6
1	B	279	THR	2.6
1	C	48	PRO	2.6
1	D	48	PRO	2.6
1	C	257	ARG	2.6
1	B	285	THR	2.6
1	A	48	PRO	2.6
1	C	246	VAL	2.5
1	D	75	ILE	2.5
1	D	163	TYR	2.5
1	A	111	ARG	2.5
1	B	249	GLY	2.5
1	C	77	ALA	2.5
1	D	248	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	395	SER	2.4
1	B	41	ALA	2.4
1	A	202	GLY	2.4
1	D	116	GLN	2.4
1	B	421	ASP	2.4
1	C	206	SER	2.4
1	D	222	SER	2.4
1	B	203	THR	2.4
1	C	43	GLU	2.4
1	C	127	GLU	2.4
1	A	508	SER	2.4
1	D	120	GLU	2.3
1	D	502	ASP	2.3
1	B	200	LEU	2.3
1	A	76	SER	2.3
1	C	42	ALA	2.3
1	C	201	TYR	2.3
1	D	509	TYR	2.3
1	B	251	CYS	2.3
1	D	44	LYS	2.3
1	A	75	ILE	2.2
1	B	207	THR	2.2
1	C	322	ASP	2.2
1	C	145	LEU	2.2
1	C	26	GLU	2.2
1	D	43	GLU	2.2
1	B	96	ASN	2.2
1	A	203	THR	2.2
1	A	78	VAL	2.2
1	D	228	VAL	2.2
1	C	225	ILE	2.2
1	D	284	THR	2.2
1	A	251	CYS	2.2
1	B	508	SER	2.2
1	C	486	ARG	2.2
1	D	508	SER	2.2
1	C	485	TYR	2.2
1	C	205	ASN	2.2
1	A	79	PRO	2.1
1	A	41	ALA	2.1
1	A	77	ALA	2.1
1	A	284	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	284	THR	2.1
1	D	82	GLY	2.1
1	A	254	LEU	2.1
1	A	170	THR	2.1
1	B	202	GLY	2.1
1	B	125	LEU	2.0
1	C	264	THR	2.0
1	B	76	SER	2.0
1	A	509	TYR	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
2	GOL	D	601	6/6	0.71	0.17	39,39,39,41	0
2	GOL	C	601	6/6	0.83	0.15	39,40,40,41	0
2	GOL	A	601	6/6	0.84	0.16	45,46,46,47	0
2	GOL	C	602	6/6	0.87	0.14	39,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.