



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2026 – 05:25 pm BST

PDB ID : 28MG / pdb\_000028mg  
Title : crystal structure of Dpo31, of a tail-spike protein with depolymerase activity identified in a marine podovirus  
Authors : Czjzek, M.; Sirigu, S.; Roret, T.; Baudoux, A.C.  
Deposited on : 2026-02-06  
Resolution : 2.15 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](mailto: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>.

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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	:	1.8.4, CSD as541be (2020)
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

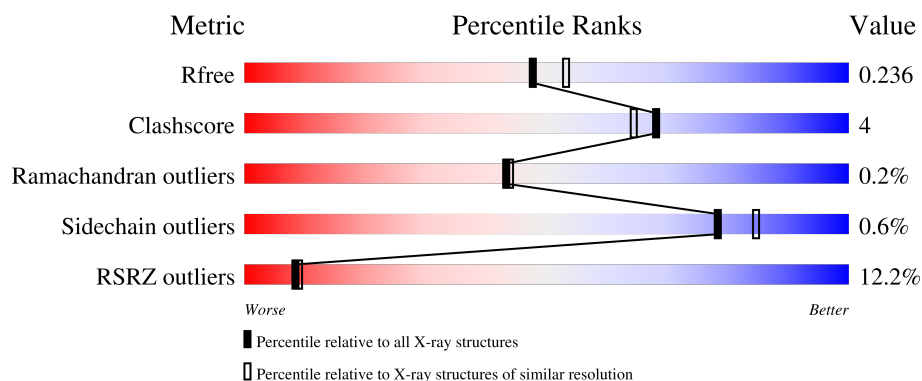
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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  $\geq 3$ , 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	828	<div> <div>9%</div> <div>61%</div> <div>5%</div> <div>33%</div> </div>
1	B	828	<div> <div>9%</div> <div>61%</div> <div>6%</div> <div>32%</div> </div>
1	C	828	<div> <div>7%</div> <div>60%</div> <div>6%</div> <div>34%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12545 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 Dpo31-deltaD1, viral depolymerase depleted of domain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	2	0
			4023	2443	703	864	13			
1	B	561	Total	C	N	O	S	0	2	0
			4101	2492	715	881	13			
1	C	545	Total	C	N	O	S	0	4	0
			3976	2417	693	854	12			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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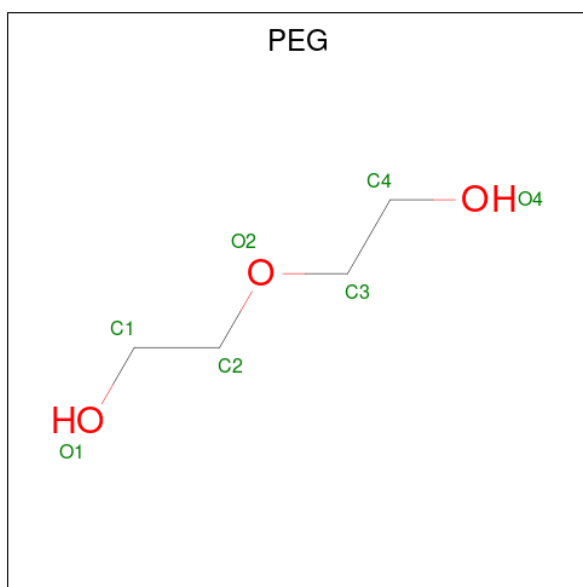
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	118	Total	O	0	0
			118	118		
5	B	135	Total	O	0	0
			135	135		

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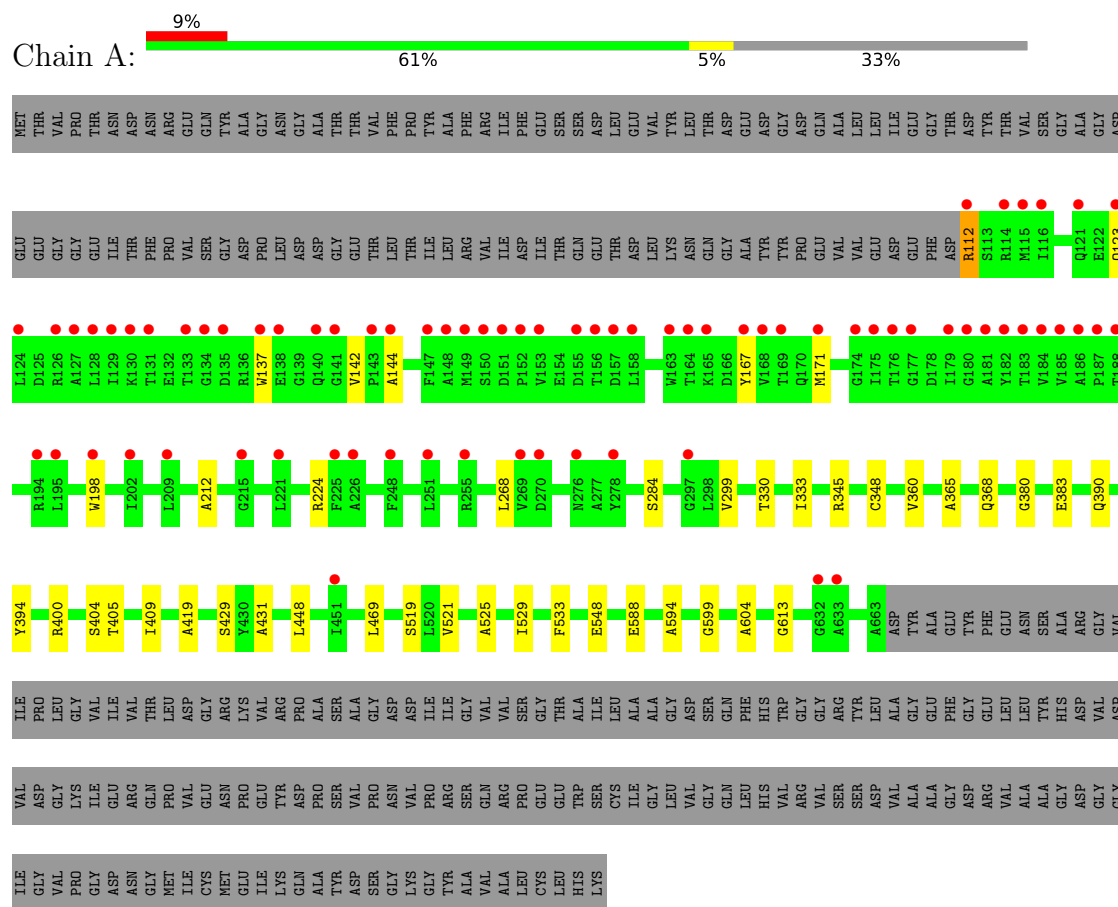
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	158	Total 158	O 158	0	0

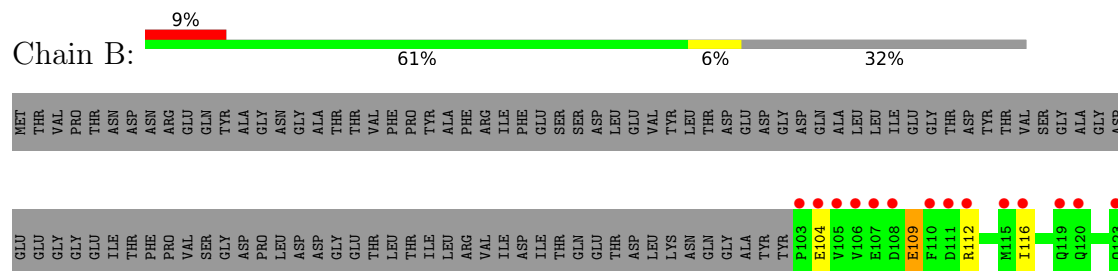
### 3 Residue-property plots

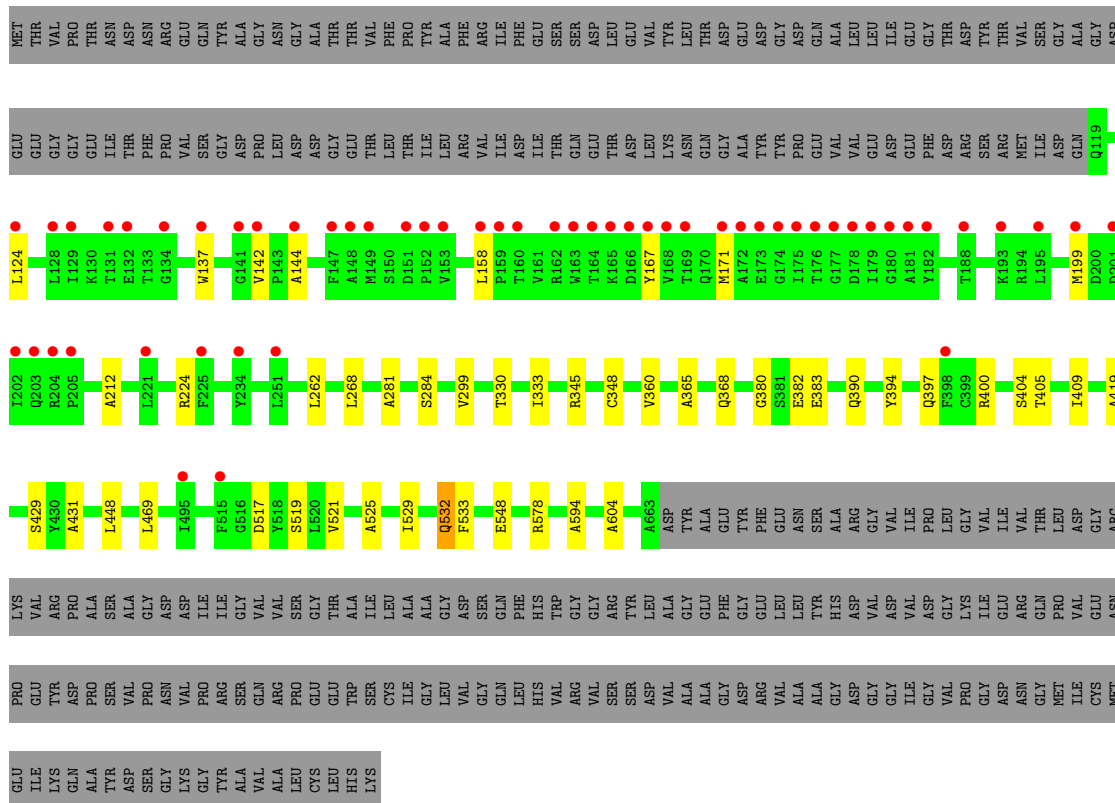
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dpo31-deltaD1, viral depolymerase depleted of domain 1



- Molecule 1: Dpo31-deltaD1, viral depolymerase depleted of domain 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.73Å 75.61Å 124.94Å 90.00° 103.30° 90.00°	Depositor
Resolution (Å)	47.38 – 2.15 47.38 – 2.15	Depositor EDS
% Data completeness (in resolution range)	63.8 (47.38-2.15) 63.7 (47.38-2.15)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.10.4 (21-NOV-2022)	Depositor
R, $R_{free}$	0.212 , 0.243 0.206 , 0.236	Depositor DCC
$R_{free}$ test set	2978 reflections (3.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG, GOL, MG

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	0.58	0/4090	0.92	0/5557
1	B	0.57	0/4170	0.93	1/5665 (0.0%)
1	C	0.58	0/4049	0.92	0/5503
All	All	0.58	0/12309	0.92	1/16725 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	HIS	N-CA-C	5.01	118.68	112.47

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	4023	0	3764	34	0
1	B	4101	0	3834	38	0
1	C	3976	0	3722	35	0
2	A	12	0	16	1	0
2	C	12	0	16	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	C	7	0	10	0	0
5	A	118	0	0	0	0
5	B	135	0	0	0	0
5	C	158	0	0	0	0
All	All	12545	0	11362	85	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 4.

All (85) 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:A:519:SER:HB2	1:A:529:ILE:HD13	1.61	0.82
1:B:519:SER:HB2	1:B:529:ILE:HD13	1.61	0.81
1:C:519:SER:HB2	1:C:529:ILE:HD13	1.60	0.81
1:A:137:TRP:NE1	1:B:142:VAL:HB	2.09	0.68
1:A:137:TRP:HE1	1:B:142:VAL:HB	1.58	0.68
1:B:137:TRP:HE1	1:C:142:VAL:HB	1.62	0.65
1:A:137:TRP:CD1	1:B:142:VAL:HG12	2.35	0.61
1:A:212:ALA:H	1:A:224:ARG:NH2	2.00	0.60
1:B:137:TRP:NE1	1:C:142:VAL:HB	2.15	0.60
1:C:212:ALA:H	1:C:224:ARG:NH2	2.01	0.58
1:B:212:ALA:H	1:B:224:ARG:NH2	2.02	0.58
1:A:519:SER:CB	1:A:529:ILE:HD13	2.33	0.57
1:C:519:SER:CB	1:C:529:ILE:HD13	2.31	0.57
1:B:519:SER:CB	1:B:529:ILE:HD13	2.34	0.56
1:B:137:TRP:CD1	1:C:142:VAL:HG12	2.40	0.55
1:C:429:SER:HB3	1:C:521:VAL:HG11	1.89	0.54
1:A:429:SER:HB3	1:A:521:VAL:HG11	1.89	0.54
1:A:448:LEU:HD22	1:A:469:LEU:HD11	1.90	0.54
1:A:330:THR:HB	1:A:345:ARG:H	1.73	0.54
1:B:429:SER:HB3	1:B:521:VAL:HG11	1.90	0.53
1:A:431:ALA:HA	1:A:529:ILE:HG13	1.90	0.53
1:C:330:THR:HB	1:C:345:ARG:H	1.73	0.53
1:A:268:LEU:HA	1:A:284:SER:HB3	1.91	0.53
1:B:448:LEU:HD22	1:B:469:LEU:HD11	1.91	0.53
1:C:382:GLU:HB3	1:C:397[B]:GLN:HG3	1.90	0.53
1:C:431:ALA:HA	1:C:529:ILE:HG13	1.91	0.53
1:C:448:LEU:HD22	1:C:469:LEU:HD11	1.91	0.53
1:C:517[B]:ASP:HB3	1:C:532[B]:GLN:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:THR:HB	1:B:345:ARG:H	1.72	0.52
1:B:268:LEU:HA	1:B:284:SER:HB3	1.91	0.52
1:C:268:LEU:HA	1:C:284:SER:HB3	1.90	0.52
1:B:431:ALA:HA	1:B:529:ILE:HG13	1.90	0.51
1:A:112:ARG:N	1:A:112:ARG:HE	2.11	0.49
1:B:390:GLN:O	1:B:405:THR:HA	2.12	0.49
1:C:368:GLN:O	1:C:383:GLU:HA	2.12	0.49
1:B:368:GLN:O	1:B:383:GLU:HA	2.13	0.49
1:A:368:GLN:O	1:A:383:GLU:HA	2.14	0.48
1:C:390:GLN:O	1:C:405:THR:HA	2.14	0.48
1:A:142:VAL:HB	1:C:137:TRP:HE1	1.78	0.48
1:B:533:PHE:CE1	1:C:525:ALA:HB2	2.49	0.47
1:A:390:GLN:O	1:A:405:THR:HA	2.14	0.47
1:C:333:ILE:HG22	1:C:348:CYS:HB2	1.97	0.47
1:B:333:ILE:HG22	1:B:348:CYS:HB2	1.97	0.46
1:A:137:TRP:CD1	1:B:142:VAL:CG1	2.99	0.46
1:A:142:VAL:HB	1:C:137:TRP:NE1	2.31	0.46
1:A:198:TRP:CG	1:C:199:MET:SD	3.08	0.46
1:A:144:ALA:HB3	1:B:158:LEU:HB2	1.98	0.46
1:A:333:ILE:HG22	1:A:348:CYS:HB2	1.98	0.46
1:B:109:GLU:HG2	1:B:112:ARG:HH21	1.81	0.46
1:B:144:ALA:HB3	1:C:158:LEU:HB2	1.99	0.45
1:B:420:HIS:NE2	1:C:397[A]:GLN:NE2	2.64	0.45
1:A:599:GLY:HA2	1:A:613:GLY:O	2.18	0.44
1:A:533:PHE:CE1	1:B:525:ALA:HB2	2.54	0.43
1:A:142:VAL:HG12	1:C:137:TRP:CD1	2.53	0.43
1:B:262:LEU:HD12	1:B:281:ALA:HB2	2.01	0.43
1:B:299:VAL:HB	1:C:333:ILE:HG13	2.01	0.43
1:A:594:ALA:HB1	1:A:604:ALA:HB1	2.01	0.43
1:B:112:ARG:HD2	1:B:116:ILE:HD12	2.00	0.43
1:A:299:VAL:HB	1:B:333:ILE:HG13	2.01	0.43
1:C:167:TYR:O	1:C:171:MET:HG2	2.19	0.43
1:B:394:TYR:O	1:B:409:ILE:HA	2.19	0.42
1:C:594:ALA:HB1	1:C:604:ALA:HB1	2.00	0.42
1:B:533:PHE:O	1:B:548:GLU:HA	2.19	0.42
1:A:525:ALA:HB2	1:C:533:PHE:CE1	2.55	0.42
1:B:594:ALA:HB1	1:B:604:ALA:HB1	2.01	0.42
1:B:359:ASN:O	1:B:374:PRO:HA	2.20	0.42
1:A:365:ALA:O	1:A:380:GLY:HA2	2.20	0.42
1:A:167:TYR:O	1:A:171:MET:HG2	2.20	0.42
1:B:137:TRP:HB2	1:C:144:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ILE:HG13	1:C:299:VAL:HB	2.02	0.41
1:C:533:PHE:O	1:C:548:GLU:HA	2.20	0.41
1:A:533:PHE:O	1:A:548:GLU:HA	2.19	0.41
1:C:262:LEU:HD12	1:C:281:ALA:HB2	2.02	0.41
1:A:588:GLU:HB2	2:A:902:GOL:H12	2.03	0.41
1:B:365:ALA:O	1:B:380:GLY:HA2	2.21	0.41
1:C:404:SER:O	1:C:419:ALA:HA	2.21	0.41
1:A:123:GLN:HB3	1:C:124:LEU:HD21	2.03	0.41
1:B:404:SER:O	1:B:419:ALA:HA	2.20	0.41
1:C:365:ALA:O	1:C:380:GLY:HA2	2.21	0.41
1:A:394:TYR:O	1:A:409:ILE:HA	2.20	0.41
1:B:599:GLY:HA2	1:B:613:GLY:O	2.21	0.40
1:C:394:TYR:O	1:C:409:ILE:HA	2.21	0.40
1:A:404:SER:O	1:A:419:ALA:HA	2.22	0.40
1:B:151:ASP:HA	1:B:152:PRO:HA	1.94	0.40
1:B:419:ALA:O	1:B:517:ASP:HA	2.21	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	552/828 (67%)	535 (97%)	16 (3%)	1 (0%)	43	44
1	B	561/828 (68%)	545 (97%)	15 (3%)	1 (0%)	43	44
1	C	547/828 (66%)	530 (97%)	16 (3%)	1 (0%)	43	44
All	All	1660/2484 (67%)	1610 (97%)	47 (3%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	360	VAL

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Mol	Chain	Res	Type
1	C	360	VAL
1	A	360	VAL

### 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	416/635 (66%)	414 (100%)	2 (0%)	81	87
1	B	425/635 (67%)	422 (99%)	3 (1%)	76	82
1	C	411/635 (65%)	407 (99%)	4 (1%)	68	75
All	All	1252/1905 (66%)	1243 (99%)	9 (1%)	78	82

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

Mol	Chain	Res	Type
1	A	112	ARG
1	A	400	ARG
1	B	104	GLU
1	B	109	GLU
1	B	400	ARG
1	C	400	ARG
1	C	532[A]	GLN
1	C	532[B]	GLN
1	C	578	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	274	ASN
1	A	393	ASN
1	A	408	ASN
1	A	563	ASN
1	B	146	ASN

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Mol	Chain	Res	Type
1	B	274	ASN
1	B	329	HIS
1	B	393	ASN
1	B	408	ASN
1	B	563	ASN
1	C	120	GLN
1	C	146	ASN
1	C	274	ASN
1	C	393	ASN
1	C	563	ASN

### 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](#)

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	$\# Z  > 2$
2	GOL	C	901	-	5,5,5	0.04	0	5,5,5	0.23	0
2	GOL	A	902	-	5,5,5	0.05	0	5,5,5	0.20	0
2	GOL	A	901	-	5,5,5	0.07	0	5,5,5	0.27	0
4	PEG	C	903	-	6,6,6	0.19	0	5,5,5	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	C	902	-	5,5,5	0.05	0	5,5,5	0.11	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	901	-	-	0/4/4/4	-
2	GOL	A	902	-	-	0/4/4/4	-
2	GOL	A	901	-	-	0/4/4/4	-
4	PEG	C	903	-	-	1/4/4/4	-
2	GOL	C	902	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	903	PEG	O2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	552/828 (66%)	0.62	74 (13%)  	17, 49, 170, 206	2 (0%)
1	B	561/828 (67%)	0.64	74 (13%)  	19, 52, 164, 179	2 (0%)
1	C	545/828 (65%)	0.43	55 (10%)  	15, 43, 165, 189	4 (0%)
All	All	1658/2484 (66%)	0.56	203 (12%)  	15, 47, 166, 206	8 (0%)

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	PRO	7.7
1	A	202	ILE	6.6
1	A	179	ILE	4.9
1	A	276	ASN	4.7
1	A	158	LEU	4.7
1	A	124	LEU	4.7
1	B	143	PRO	4.7
1	A	195	LEU	4.5
1	B	110	PHE	4.2
1	B	481	VAL	4.2
1	A	147	PHE	4.2
1	A	148	ALA	4.2
1	A	181	ALA	4.2
1	A	156	THR	4.1
1	A	133	THR	4.1
1	B	175	ILE	4.1
1	C	179	ILE	4.1
1	A	632	GLY	4.0
1	B	148	ALA	3.9
1	A	175	ILE	3.9
1	B	141	GLY	3.9
1	B	184	VAL	3.8
1	B	128	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	513	ASP	3.7
1	A	185	VAL	3.7
1	C	128	LEU	3.7
1	A	152	PRO	3.7
1	A	184	VAL	3.7
1	A	137	TRP	3.6
1	C	205	PRO	3.6
1	C	153	VAL	3.6
1	A	129	ILE	3.6
1	A	226	ALA	3.6
1	B	104	GLU	3.6
1	C	175	ILE	3.6
1	C	172	ALA	3.5
1	A	128	LEU	3.5
1	A	163	TRP	3.5
1	A	153	VAL	3.5
1	B	183	THR	3.5
1	A	198	TRP	3.4
1	C	142	VAL	3.4
1	C	169	THR	3.4
1	A	180	GLY	3.4
1	B	515	PHE	3.4
1	A	182	TYR	3.4
1	B	182	TYR	3.4
1	C	131	THR	3.4
1	C	162	ARG	3.3
1	A	167	TYR	3.3
1	B	105	VAL	3.3
1	B	235	GLY	3.3
1	B	144	ALA	3.3
1	A	221	LEU	3.3
1	C	203	GLN	3.3
1	C	199	MET	3.3
1	A	269	VAL	3.3
1	A	115	MET	3.3
1	C	177	GLY	3.2
1	B	439	GLY	3.2
1	C	176	THR	3.2
1	C	165	LYS	3.2
1	C	182	TYR	3.1
1	A	215	GLY	3.1
1	C	178	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	129	ILE	3.1
1	B	209	LEU	3.1
1	A	183	THR	3.1
1	A	278	TYR	3.1
1	C	234	TYR	3.1
1	C	180	GLY	3.1
1	B	158	LEU	3.1
1	B	115	MET	3.1
1	C	158	LEU	3.0
1	C	174	GLY	3.0
1	C	148	ALA	2.9
1	A	150	SER	2.9
1	B	142	VAL	2.9
1	B	188	THR	2.9
1	B	446	GLY	2.9
1	B	106	VAL	2.9
1	A	176	THR	2.9
1	C	188	THR	2.9
1	B	147	PHE	2.9
1	A	633	ALA	2.9
1	C	129	ILE	2.8
1	C	251	LEU	2.8
1	C	152	PRO	2.8
1	B	112	ARG	2.8
1	C	181	ALA	2.8
1	B	153	VAL	2.8
1	A	451	ILE	2.8
1	B	463	GLY	2.8
1	C	168	VAL	2.8
1	A	174	GLY	2.7
1	A	127	ALA	2.7
1	A	144	ALA	2.7
1	A	164	THR	2.7
1	B	108	ASP	2.7
1	C	137	TRP	2.7
1	B	149	MET	2.7
1	A	151	ASP	2.7
1	A	297	GLY	2.7
1	A	131	THR	2.6
1	B	133	THR	2.6
1	C	159	PRO	2.6
1	C	166	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	491	GLY	2.6
1	C	171	MET	2.6
1	C	193	LYS	2.6
1	B	164	THR	2.6
1	C	144	ALA	2.6
1	C	164	THR	2.6
1	A	116	ILE	2.6
1	B	168	VAL	2.6
1	B	240	GLY	2.6
1	B	172	ALA	2.6
1	B	137	TRP	2.6
1	C	147	PHE	2.5
1	B	318	ASN	2.5
1	B	136	ARG	2.5
1	C	201	ASP	2.5
1	A	186	ALA	2.5
1	C	149	MET	2.5
1	A	123	GLN	2.5
1	B	132	GLU	2.5
1	C	124	LEU	2.5
1	A	112	ARG	2.5
1	B	131	THR	2.5
1	A	248	PHE	2.5
1	B	198	TRP	2.5
1	C	163	TRP	2.5
1	B	499	ASP	2.4
1	B	510	ALA	2.4
1	C	221	LEU	2.4
1	C	398	PHE	2.4
1	A	138	GLU	2.4
1	B	140	GLN	2.4
1	B	482	ILE	2.4
1	B	156	THR	2.4
1	A	134	GLY	2.4
1	A	155	ASP	2.4
1	B	116	ILE	2.4
1	A	114	ARG	2.4
1	C	167	TYR	2.3
1	B	127	ALA	2.3
1	A	121	GLN	2.3
1	B	124	LEU	2.3
1	A	188	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	169	THR	2.3
1	B	176	THR	2.3
1	B	134	GLY	2.3
1	C	141	GLY	2.3
1	B	437	PHE	2.3
1	C	225	PHE	2.3
1	B	236	ILE	2.3
1	A	209	LEU	2.3
1	A	165	LYS	2.3
1	C	515	PHE	2.3
1	B	111	ASP	2.3
1	B	178	ASP	2.3
1	A	177	GLY	2.3
1	A	140	GLN	2.2
1	B	119	GLN	2.2
1	A	168	VAL	2.2
1	C	160	THR	2.2
1	A	251	LEU	2.2
1	C	173	GLU	2.2
1	A	194	ARG	2.2
1	A	169	THR	2.2
1	C	202	ILE	2.2
1	C	495	ILE	2.2
1	B	316	VAL	2.2
1	A	157	ASP	2.2
1	A	141	GLY	2.2
1	A	187	PRO	2.2
1	C	134	GLY	2.2
1	B	195	LEU	2.2
1	A	135	ASP	2.2
1	A	143	PRO	2.1
1	B	159	PRO	2.1
1	C	151	ASP	2.2
1	C	132	GLU	2.1
1	B	161	VAL	2.1
1	B	123	GLN	2.1
1	A	255	ARG	2.1
1	C	195	LEU	2.1
1	B	171	MET	2.1
1	B	479	ASP	2.1
1	B	488	GLY	2.1
1	B	212	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	145	LYS	2.1
1	B	498	THR	2.1
1	A	225	PHE	2.1
1	A	270	ASP	2.1
1	A	126	ARG	2.1
1	C	204	ARG	2.1
1	A	171	MET	2.0
1	B	107	GLU	2.0
1	A	149	MET	2.0
1	B	274	ASN	2.0
1	B	120	GLN	2.0
1	A	130	LYS	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, 95<sup>th</sup> 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	C	901	6/6	0.81	0.17	95,96,96,96	0
3	MG	A	903	1/1	0.83	0.07	38,38,38,38	0
2	GOL	C	902	6/6	0.87	0.10	57,57,57,57	0
4	PEG	C	903	7/7	0.87	0.19	66,67,69,69	0
2	GOL	A	901	6/6	0.89	0.15	70,70,71,71	0
2	GOL	A	902	6/6	0.90	0.13	73,73,74,74	0
3	MG	B	901	1/1	0.96	0.09	43,43,43,43	0
3	MG	C	904	1/1	0.97	0.03	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.