



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:33 PM UTC

PDB ID : 2DDB / pdb\_00002ddb  
Title : Crystal structure of pseudecin from Pseudechis porphyriacus  
Authors : Suzuki, N.; Yamazaki, Y.; Fujimoto, Z.; Morita, T.; Mizuno, H.  
Deposited on : 2006-01-25  
Resolution : 1.90 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 : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

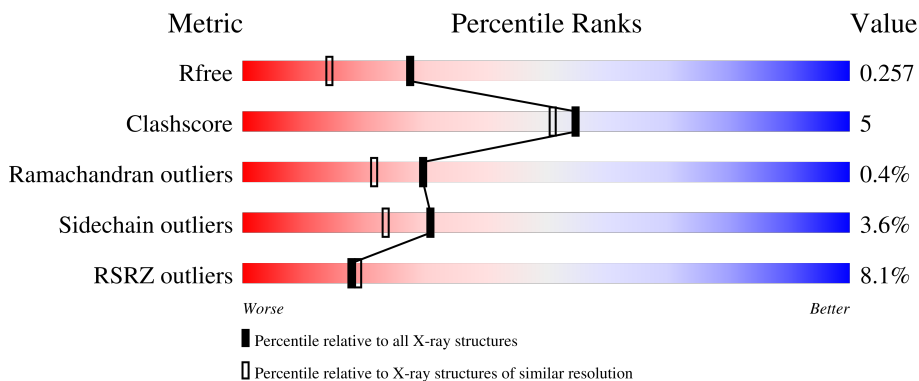
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


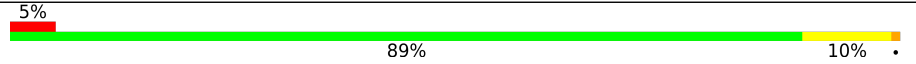
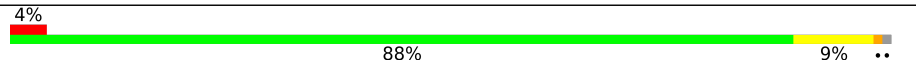

The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	210	 6% 88% 10% ..
1	B	210	 5% 89% 10% .
1	C	210	 4% 88% 9% ..
1	D	210	 16% 88% 10% .

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7362 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 Pseudecin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	1627	1023	298	287	19	0	1	0
1	B	209	1645	1035	302	289	19	0	1	0
1	C	207	1624	1022	296	287	19	0	0	0
1	D	209	1642	1034	300	289	19	0	0	0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

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

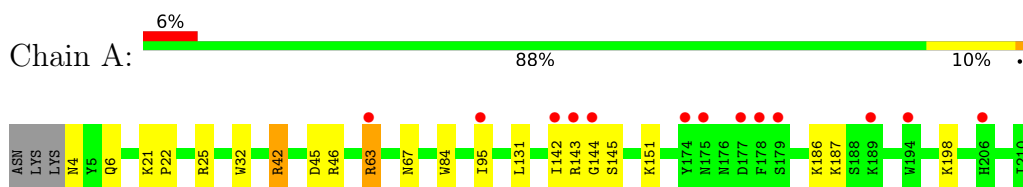
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	201	Total	O	0	0
			201	201		
5	B	172	Total	O	0	0
			172	172		
5	C	219	Total	O	0	0
			219	219		
5	D	129	Total	O	0	0
			129	129		

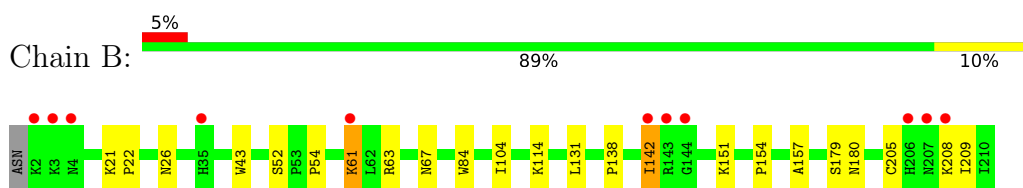
### 3 Residue-property plots [i](#)

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.

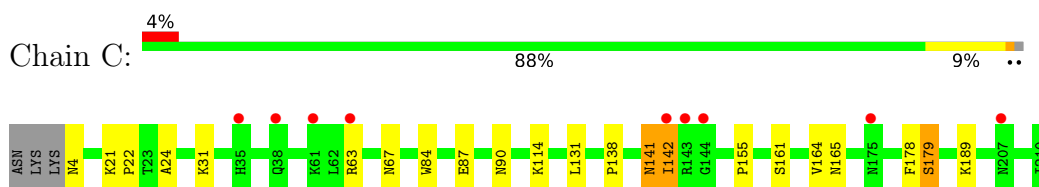
- Molecule 1: Pseudecin



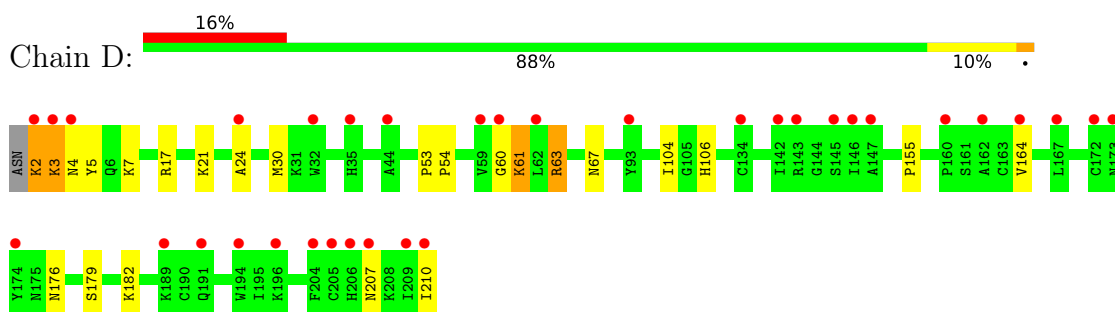
- Molecule 1: Pseudecin



- Molecule 1: Pseudecin



- Molecule 1: Pseudecin



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.71Å 61.67Å 251.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.27 – 1.90 43.27 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.27-1.90) 98.4 (43.27-1.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.51 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.206 , 0.258 0.206 , 0.257	Depositor DCC
$R_{free}$ test set	3745 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtrriage
Anisotropy	0.060	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.018 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7362	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: FMT, NA, 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	0.58	0/1682	0.81	0/2276
1	B	0.55	0/1700	0.77	0/2298
1	C	0.58	0/1671	0.78	1/2262 (0.0%)
1	D	0.50	0/1689	0.78	0/2284
All	All	0.55	0/6742	0.79	1/9120 (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	C	141	ASN	N-CA-C	5.50	119.28	112.58

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	1627	0	1578	19	0
1	B	1645	0	1604	16	0
1	C	1624	0	1581	20	0
1	D	1642	0	1607	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	21	0	7	0	0
3	B	6	0	2	0	0
3	C	24	0	8	0	0
3	D	12	0	4	0	0
4	A	18	0	24	1	0
4	C	6	0	6	0	0
4	D	12	0	15	4	0
5	A	201	0	0	4	1
5	B	172	0	0	1	0
5	C	219	0	0	7	0
5	D	129	0	0	0	0
All	All	7362	0	6436	63	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (63) 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:63:ARG:HG3	1:A:63:ARG:HH11	1.24	1.00
1:B:179:SER:HB2	1:C:142:ILE:HG22	1.45	0.98
1:A:63:ARG:HH11	1:A:63:ARG:CG	2.04	0.67
1:A:63:ARG:HG3	1:A:63:ARG:NH1	2.04	0.65
1:B:205:CYS:HB3	1:B:208:LYS:HB2	1.86	0.57
1:A:142:ILE:HG22	1:A:143:ARG:N	2.19	0.57
1:C:142:ILE:HG23	5:C:1121:HOH:O	2.03	0.57
1:A:142:ILE:HG22	1:A:143:ARG:HG2	1.87	0.57
1:D:2:LYS:O	1:D:2:LYS:HD2	2.04	0.57
1:C:114:LYS:HG3	1:C:138:PRO:HG2	1.88	0.56
1:B:114:LYS:HG3	1:B:138:PRO:HG2	1.88	0.56
1:C:31:LYS:NZ	5:C:872:HOH:O	2.35	0.55
1:C:189:LYS:NZ	5:C:627:HOH:O	2.40	0.55
1:B:179:SER:HB2	1:C:142:ILE:CG2	2.30	0.54
5:A:543:HOH:O	1:C:189:LYS:HE2	2.08	0.54
1:A:25:ARG:HD3	1:A:151:LYS:HG2	1.89	0.53
1:A:46:ARG:NH2	5:A:1066:HOH:O	2.35	0.53
1:D:54:PRO:HB3	1:D:63:ARG:NH1	2.23	0.53
1:A:21:LYS:HA	1:A:22:PRO:C	2.33	0.52
1:B:63:ARG:NH2	5:C:1105:HOH:O	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HD2	5:A:566:HOH:O	2.11	0.51
1:D:24:ALA:O	1:D:155:PRO:HA	2.11	0.49
1:B:21:LYS:HA	1:B:22:PRO:C	2.37	0.49
1:C:21:LYS:HA	1:C:22:PRO:C	2.38	0.48
1:A:4:ASN:OD1	5:A:1103:HOH:O	2.20	0.48
1:B:61:LYS:H	1:B:61:LYS:HD2	1.78	0.48
1:D:176:ASN:HD21	1:D:210:ILE:HD11	1.77	0.48
1:C:87:GLU:HG2	4:D:327:GOL:H32	1.96	0.48
1:C:87:GLU:HG2	4:D:327:GOL:H11	1.96	0.47
1:A:63:ARG:CG	1:A:63:ARG:NH1	2.69	0.47
1:B:154:PRO:HB2	1:B:157:ALA:HB2	1.96	0.47
1:B:63:ARG:HG2	5:B:1091:HOH:O	2.14	0.46
1:B:43:TRP:CD2	1:B:52:SER:HB3	2.50	0.46
1:C:24:ALA:O	1:C:155:PRO:HA	2.16	0.46
1:D:3:LYS:HD2	1:D:7:LYS:HD3	1.98	0.46
1:B:142:ILE:HG13	1:C:179:SER:HB2	1.99	0.44
1:D:176:ASN:ND2	1:D:210:ILE:HD11	2.33	0.44
1:B:43:TRP:CG	1:B:52:SER:HB3	2.53	0.44
1:A:6:GLN:HG2	1:A:32:TRP:CZ2	2.53	0.43
1:B:26:ASN:HB2	1:B:209:ILE:HD12	2.00	0.43
1:D:17:ARG:NH1	1:D:30:MET:HE3	2.34	0.43
1:A:187:LYS:NZ	1:A:187:LYS:HB3	2.34	0.43
1:A:67:ASN:HB3	1:A:84:TRP:CE2	2.54	0.42
1:B:67:ASN:HB3	1:B:84:TRP:CE2	2.55	0.42
1:C:4:ASN:N	5:C:1106:HOH:O	2.52	0.42
1:D:5:TYR:CZ	4:D:329:GOL:H12	2.54	0.42
1:D:3:LYS:H	1:D:3:LYS:HG2	1.61	0.42
1:A:45:ASP:OD2	4:A:330:GOL:O3	2.25	0.41
1:D:5:TYR:CE2	4:D:329:GOL:H31	2.55	0.41
1:D:61:LYS:HD2	1:D:61:LYS:H	1.85	0.41
1:B:54:PRO:HG2	1:C:178:PHE:CZ	2.56	0.41
1:C:142:ILE:H	1:C:142:ILE:HG12	1.55	0.41
1:B:180:ASN:HB3	1:C:141:ASN:O	2.20	0.41
1:C:67:ASN:HB3	1:C:84:TRP:CE2	2.55	0.41
1:C:164:VAL:O	1:C:165:ASN:C	2.64	0.41
1:D:67:ASN:HD21	1:D:106:HIS:HA	1.86	0.41
1:C:63:ARG:NH2	5:C:1075:HOH:O	2.54	0.40
1:C:90:ASN:ND2	5:C:987:HOH:O	2.44	0.40
1:D:53:PRO:HA	1:D:54:PRO:HD3	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:566:HOH:O	5:A:1065:HOH:O[4_556]	2.12	0.08

### 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	206/210 (98%)	199 (97%)	5 (2%)	2 (1%)	12	5
1	B	208/210 (99%)	203 (98%)	5 (2%)	0	100	100
1	C	205/210 (98%)	200 (98%)	5 (2%)	0	100	100
1	D	207/210 (99%)	203 (98%)	3 (1%)	1 (0%)	24	16
All	All	826/840 (98%)	805 (98%)	18 (2%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	SER
1	D	60	GLY
1	A	144	GLY

#### 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	180/182 (99%)	173 (96%)	7 (4%)	28	21
1	B	182/182 (100%)	177 (97%)	5 (3%)	39	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	179/182 (98%)	175 (98%)	4 (2%)	45	42
1	D	181/182 (100%)	170 (94%)	11 (6%)	17	9
All	All	722/728 (99%)	695 (96%)	27 (4%)	31	22

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42[A]	ARG
1	A	42[B]	ARG
1	A	63	ARG
1	A	95	ILE
1	A	131	LEU
1	A	186	LYS
1	A	198	LYS
1	B	61	LYS
1	B	104	ILE
1	B	131	LEU
1	B	142	ILE
1	B	151	LYS
1	C	131	LEU
1	C	142	ILE
1	C	161	SER
1	C	179	SER
1	D	2	LYS
1	D	3	LYS
1	D	4	ASN
1	D	21	LYS
1	D	61	LYS
1	D	63	ARG
1	D	104	ILE
1	D	164	VAL
1	D	179	SER
1	D	182	LYS
1	D	207	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	67	ASN

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Mol	Chain	Res	Type
1	A	173	ASN
1	A	175	ASN
1	A	206	HIS
1	B	4	ASN
1	B	55	ASN
1	B	67	ASN
1	B	90	ASN
1	B	191	GLN
1	C	67	ASN
1	C	90	ASN
1	C	206	HIS
1	D	67	ASN
1	D	90	ASN
1	D	116	HIS
1	D	173	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 31 ligands modelled in this entry, 4 are monoatomic - leaving 27 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
3	FMT	A	314	-	2,2,2	0.72	0	1,1,1	0.20	0
3	FMT	A	315	-	2,2,2	0.67	0	1,1,1	0.23	0
3	FMT	D	311	-	2,2,2	0.86	0	1,1,1	0.25	0
4	GOL	D	327	2	5,5,5	0.35	0	5,5,5	0.53	0
3	FMT	C	313	-	2,2,2	0.68	0	1,1,1	0.14	0
3	FMT	D	320	-	2,2,2	0.72	0	1,1,1	0.15	0
3	FMT	B	307	-	2,2,2	1.02	0	1,1,1	0.46	0
3	FMT	C	321	-	2,2,2	0.91	0	1,1,1	0.42	0
3	FMT	A	305	-	2,2,2	0.88	0	1,1,1	0.41	0
3	FMT	A	324	-	2,2,2	0.71	0	1,1,1	0.22	0
3	FMT	A	316	-	2,2,2	0.85	0	1,1,1	0.14	0
3	FMT	D	322	-	2,2,2	0.81	0	1,1,1	0.31	0
4	GOL	A	328	-	5,5,5	0.37	0	5,5,5	0.41	0
4	GOL	C	326	2	5,5,5	0.32	0	5,5,5	0.27	0
3	FMT	B	308	-	2,2,2	0.77	0	1,1,1	0.30	0
4	GOL	A	331	-	5,5,5	0.36	0	5,5,5	0.47	0
3	FMT	C	319	-	2,2,2	0.74	0	1,1,1	0.19	0
3	FMT	C	323	-	2,2,2	0.71	0	1,1,1	0.31	0
3	FMT	A	317	-	2,2,2	0.65	0	1,1,1	0.24	0
3	FMT	A	306	-	2,2,2	0.71	0	1,1,1	0.24	0
3	FMT	C	325	-	2,2,2	0.69	0	1,1,1	0.18	0
3	FMT	C	318	-	2,2,2	0.70	0	1,1,1	0.23	0
3	FMT	C	309	-	2,2,2	0.91	0	1,1,1	0.32	0
3	FMT	C	310	-	2,2,2	0.79	0	1,1,1	0.33	0
4	GOL	D	329	-	5,5,5	0.42	0	5,5,5	0.29	0
3	FMT	D	312	-	2,2,2	0.74	0	1,1,1	0.24	0
4	GOL	A	330	-	5,5,5	0.51	0	5,5,5	1.04	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
4	GOL	A	328	-	-	0/4/4/4	-
4	GOL	C	326	2	-	2/4/4/4	-
4	GOL	D	329	-	-	4/4/4/4	-
4	GOL	A	330	-	-	0/4/4/4	-
4	GOL	D	327	2	-	4/4/4/4	-
4	GOL	A	331	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	331	GOL	O1-C1-C2-O2
4	A	331	GOL	O1-C1-C2-C3
4	D	327	GOL	C1-C2-C3-O3
4	D	329	GOL	O1-C1-C2-C3
4	D	329	GOL	C1-C2-C3-O3
4	A	331	GOL	O2-C2-C3-O3
4	D	327	GOL	O2-C2-C3-O3
4	A	331	GOL	C1-C2-C3-O3
4	C	326	GOL	C1-C2-C3-O3
4	D	329	GOL	O1-C1-C2-O2
4	D	329	GOL	O2-C2-C3-O3
4	D	327	GOL	O1-C1-C2-C3
4	C	326	GOL	O2-C2-C3-O3
4	D	327	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	327	GOL	2	0
4	D	329	GOL	2	0
4	A	330	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	207/210 (98%)	0.28	13 (6%) 26 27	11, 20, 35, 40	1 (0%)
1	B	209/210 (99%)	0.50	11 (5%) 32 34	14, 25, 36, 49	1 (0%)
1	C	207/210 (98%)	0.26	9 (4%) 40 42	13, 21, 30, 39	0
1	D	209/210 (99%)	1.18	34 (16%) 4 4	17, 33, 42, 51	0
All	All	832/840 (99%)	0.56	67 (8%) 18 19	11, 25, 39, 51	2 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	ILE	5.3
1	C	142	ILE	4.6
1	A	142	ILE	4.1
1	C	175	ASN	4.0
1	B	143[A]	ARG	4.0
1	D	209	ILE	4.0
1	B	144	GLY	3.9
1	C	144	GLY	3.9
1	D	205	CYS	3.8
1	B	206	HIS	3.7
1	A	144	GLY	3.5
1	D	145	SER	3.5
1	D	206	HIS	3.4
1	B	2	LYS	3.3
1	B	207	ASN	3.2
1	B	3	LYS	3.1
1	D	162	ALA	3.1
1	A	178	PHE	3.1
1	A	174	TYR	3.1
1	A	177	ASP	3.1
1	D	142	ILE	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	160	PRO	3.1
1	D	147	ALA	3.0
1	D	59	VAL	3.0
1	A	143	ARG	3.0
1	A	175	ASN	3.0
1	D	3	LYS	2.8
1	D	174	TYR	2.7
1	B	4	ASN	2.7
1	A	206	HIS	2.7
1	D	62	LEU	2.7
1	C	143	ARG	2.7
1	D	204	PHE	2.7
1	D	210	ILE	2.7
1	D	134	CYS	2.6
1	D	191	GLN	2.6
1	C	35	HIS	2.5
1	A	194	TRP	2.5
1	D	173	ASN	2.4
1	D	167	LEU	2.4
1	C	63	ARG	2.4
1	D	35	HIS	2.4
1	D	194	TRP	2.3
1	C	38	GLN	2.3
1	D	32	TRP	2.3
1	B	35	HIS	2.3
1	D	2	LYS	2.3
1	D	44	ALA	2.2
1	D	146	ILE	2.2
1	D	164	VAL	2.2
1	B	61	LYS	2.2
1	D	189	LYS	2.2
1	D	60	GLY	2.1
1	C	61	LYS	2.1
1	A	63	ARG	2.1
1	B	208	LYS	2.1
1	C	207	ASN	2.1
1	A	179	SER	2.1
1	D	4	ASN	2.1
1	D	207	ASN	2.1
1	D	172	CYS	2.1
1	D	24	ALA	2.1
1	A	95	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	189	LYS	2.0
1	D	93	TYR	2.0
1	D	143	ARG	2.0
1	D	196	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(Å <sup>2</sup> )	Q<0.9
3	FMT	C	325	3/3	0.76	0.17	44,44,45,45	0
4	GOL	D	329	6/6	0.78	0.15	45,46,46,46	0
3	FMT	A	317	3/3	0.79	0.16	39,39,40,40	0
3	FMT	C	318	3/3	0.79	0.14	47,47,47,48	0
3	FMT	A	324	3/3	0.80	0.12	57,57,58,58	0
4	GOL	A	331	6/6	0.82	0.14	41,42,43,43	0
3	FMT	C	313	3/3	0.83	0.15	41,41,41,41	0
4	GOL	A	330	6/6	0.83	0.17	28,31,34,37	0
3	FMT	A	314	3/3	0.84	0.13	37,37,38,38	0
3	FMT	C	319	3/3	0.84	0.17	49,49,49,49	0
3	FMT	C	323	3/3	0.85	0.11	36,36,37,37	0
3	FMT	D	320	3/3	0.87	0.13	41,41,41,42	0
3	FMT	C	321	3/3	0.87	0.14	35,35,35,35	0
4	GOL	C	326	6/6	0.89	0.14	25,26,27,30	0
3	FMT	A	305	3/3	0.90	0.15	37,37,38,38	0
4	GOL	A	328	6/6	0.90	0.10	31,33,34,36	0
3	FMT	A	315	3/3	0.92	0.10	23,23,25,26	0
3	FMT	D	312	3/3	0.92	0.09	37,37,37,37	0
3	FMT	A	316	3/3	0.92	0.10	28,28,30,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	D	327	6/6	0.92	0.10	24,28,31,31	0
3	FMT	A	306	3/3	0.92	0.18	32,32,33,33	0
3	FMT	D	322	3/3	0.93	0.09	34,34,34,35	0
3	FMT	D	311	3/3	0.94	0.10	26,26,26,27	0
3	FMT	B	307	3/3	0.95	0.07	19,19,20,22	0
2	NA	C	302	1/1	0.96	0.05	20,20,20,20	0
3	FMT	B	308	3/3	0.96	0.07	21,21,22,23	0
3	FMT	C	309	3/3	0.96	0.07	26,26,26,27	0
3	FMT	C	310	3/3	0.96	0.08	25,25,26,26	0
2	NA	B	303	1/1	0.97	0.05	20,20,20,20	0
2	NA	D	304	1/1	0.98	0.03	18,18,18,18	0
2	NA	A	301	1/1	1.00	0.01	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.