



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 05:52 am GMT

PDB ID : 5OCR  
Title : Crystal structure of the kappa-carrageenase zobellia\_236 from *Zobellia galactanivorans*  
Authors : Czjzek, M.; Matard-Mann, M.; Michel, G.; Jeudy, A.; Larocque, R.  
Deposited on : 2017-07-03  
Resolution : 1.66 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

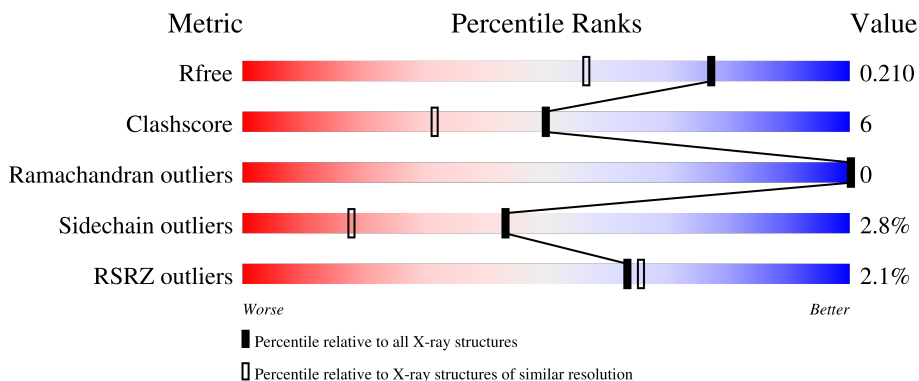
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.66 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))
$R_{free}$	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	286	 82% 14% ..
1	B	286	 80% 15% ..
1	C	286	 83% 13% ..
1	D	286	 84% 10% ...

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 10456 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 Kappa-carrageenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	278	Total 2411	C 1551	N 403	O 449	S 8	0	20	0
1	B	278	Total 2399	C 1543	N 398	O 450	S 8	0	17	0
1	C	278	Total 2395	C 1542	N 396	O 449	S 8	0	17	0
1	D	278	Total 2427	C 1561	N 407	O 451	S 8	0	20	0

There are 44 discrepancies between the modelled and reference sequences:

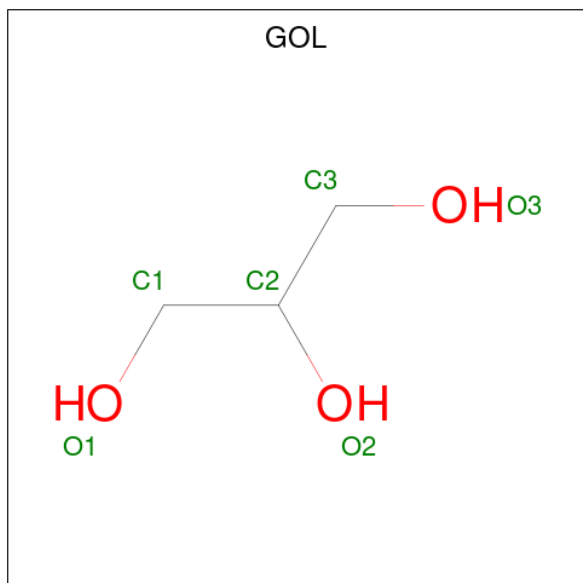
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	HIS	-	expression tag	UNP O84907
A	23	HIS	-	expression tag	UNP O84907
A	24	HIS	-	expression tag	UNP O84907
A	25	HIS	-	expression tag	UNP O84907
A	26	HIS	-	expression tag	UNP O84907
A	27	HIS	-	expression tag	UNP O84907
A	28	GLY	-	expression tag	UNP O84907
A	29	SER	-	expression tag	UNP O84907
A	?	-	PRO	deletion	UNP O84907
A	214	PRO	-	insertion	UNP O84907
A	215	TRP	MET	conflict	UNP O84907
B	22	HIS	-	expression tag	UNP O84907
B	23	HIS	-	expression tag	UNP O84907
B	24	HIS	-	expression tag	UNP O84907
B	25	HIS	-	expression tag	UNP O84907
B	26	HIS	-	expression tag	UNP O84907
B	27	HIS	-	expression tag	UNP O84907
B	28	GLY	-	expression tag	UNP O84907
B	29	SER	-	expression tag	UNP O84907
B	?	-	PRO	deletion	UNP O84907
B	214	PRO	-	insertion	UNP O84907

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Chain	Residue	Modelled	Actual	Comment	Reference
B	215	TRP	MET	conflict	UNP O84907
C	22	HIS	-	expression tag	UNP O84907
C	23	HIS	-	expression tag	UNP O84907
C	24	HIS	-	expression tag	UNP O84907
C	25	HIS	-	expression tag	UNP O84907
C	26	HIS	-	expression tag	UNP O84907
C	27	HIS	-	expression tag	UNP O84907
C	28	GLY	-	expression tag	UNP O84907
C	29	SER	-	expression tag	UNP O84907
C	?	-	PRO	deletion	UNP O84907
C	214	PRO	-	insertion	UNP O84907
C	215	TRP	MET	conflict	UNP O84907
D	22	HIS	-	expression tag	UNP O84907
D	23	HIS	-	expression tag	UNP O84907
D	24	HIS	-	expression tag	UNP O84907
D	25	HIS	-	expression tag	UNP O84907
D	26	HIS	-	expression tag	UNP O84907
D	27	HIS	-	expression tag	UNP O84907
D	28	GLY	-	expression tag	UNP O84907
D	29	SER	-	expression tag	UNP O84907
D	?	-	PRO	deletion	UNP O84907
D	214	PRO	-	insertion	UNP O84907
D	215	TRP	MET	conflict	UNP O84907

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

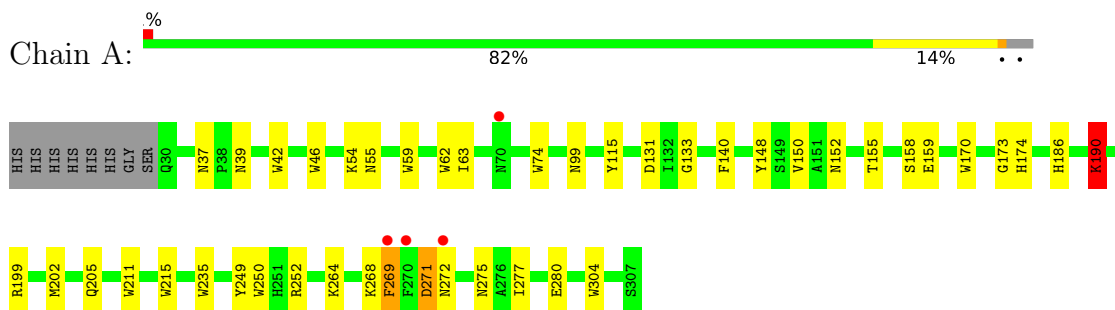
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	221	Total	O	0	0
			221	221		
4	B	180	Total	O	0	0
			180	180		
4	C	177	Total	O	0	0
			177	177		
4	D	202	Total	O	0	0
			202	202		

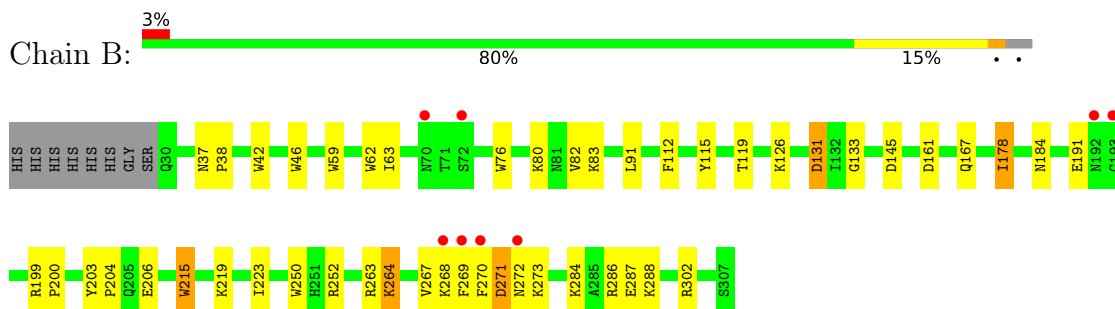
### 3 Residue-property plots [i](#)

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.

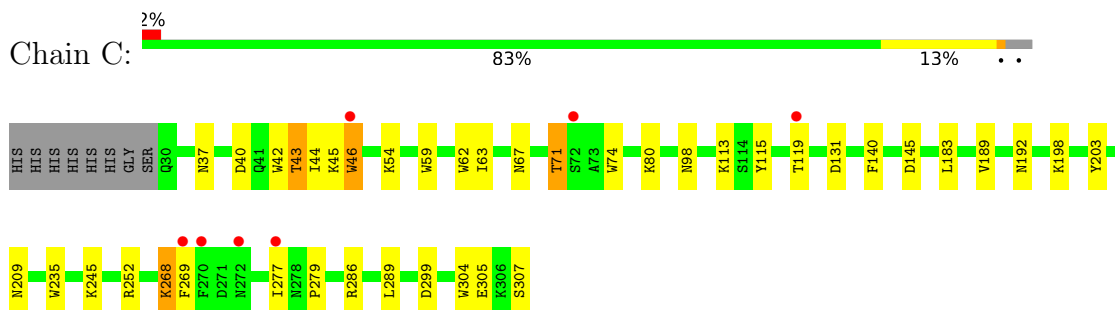
- Molecule 1: Kappa-carrageenase



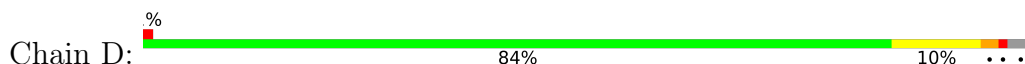
- Molecule 1: Kappa-carrageenase

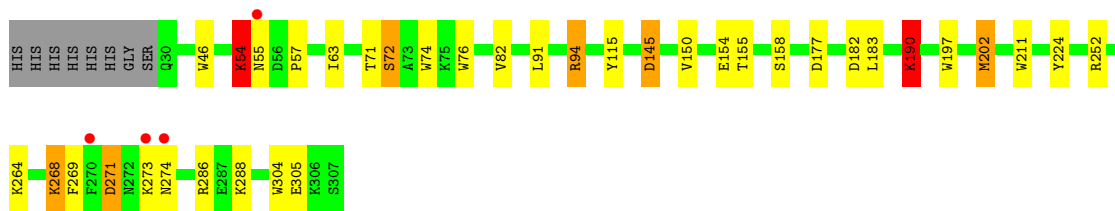


- Molecule 1: Kappa-carrageenase



- Molecule 1: Kappa-carrageenase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.96Å 83.04Å 85.71Å 72.56° 88.34° 89.48°	Depositor
Resolution (Å)	81.74 – 1.66 79.22 – 1.66	Depositor EDS
% Data completeness (in resolution range)	94.2 (81.74-1.66) 94.2 (79.22-1.66)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 1.66Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.168 , 0.206 0.172 , 0.210	Depositor DCC
$R_{free}$ test set	5681 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.096 for h,-k,-l 0.000 for -h,l,k 0.000 for -h,-l,-k	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10456	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2104e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 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	1.20	10/2545 (0.4%)	1.06	4/3457 (0.1%)
1	B	1.15	7/2527 (0.3%)	1.07	8/3435 (0.2%)
1	C	1.13	8/2517 (0.3%)	1.03	4/3425 (0.1%)
1	D	1.18	9/2558 (0.4%)	1.10	9/3476 (0.3%)
All	All	1.17	34/10147 (0.3%)	1.07	25/13793 (0.2%)

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
1	A	0	1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	TRP	CD2-CE2	6.85	1.49	1.41
1	B	62	TRP	CD2-CE2	6.72	1.49	1.41
1	C	59	TRP	CD2-CE2	6.69	1.49	1.41
1	B	59	TRP	CD2-CE2	6.66	1.49	1.41
1	A	74	TRP	CD2-CE2	6.65	1.49	1.41
1	D	211	TRP	CD2-CE2	6.26	1.48	1.41
1	A	42	TRP	CD2-CE2	6.12	1.48	1.41
1	A	211	TRP	CD2-CE2	6.10	1.48	1.41
1	C	62	TRP	CD2-CE2	6.00	1.48	1.41
1	C	62	TRP	CG-CD1	5.98	1.45	1.36
1	B	42	TRP	CD2-CE2	5.86	1.48	1.41
1	B	46	TRP	CD2-CE2	5.76	1.48	1.41
1	A	304	TRP	CD2-CE2	5.67	1.48	1.41
1	D	76	TRP	CD2-CE2	5.59	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	54	LYS	N-CA	5.56	1.57	1.46
1	C	235	TRP	CD2-CE2	5.51	1.48	1.41
1	D	224	TYR	CG-CD2	5.41	1.46	1.39
1	D	158	SER	CA-CB	5.38	1.61	1.52
1	A	46	TRP	CG-CD1	5.33	1.44	1.36
1	D	197	TRP	CD2-CE2	5.33	1.47	1.41
1	A	46	TRP	CD2-CE2	5.28	1.47	1.41
1	C	46	TRP	CD2-CE2	5.26	1.47	1.41
1	C	74	TRP	CD2-CE2	5.24	1.47	1.41
1	C	42	TRP	CD2-CE2	5.24	1.47	1.41
1	A	59	TRP	CD2-CE2	5.24	1.47	1.41
1	D	74	TRP	CD2-CE2	5.20	1.47	1.41
1	C	304	TRP	CD2-CE2	5.17	1.47	1.41
1	B	250	TRP	CD2-CE2	5.15	1.47	1.41
1	B	215	TRP	CG-CD2	5.13	1.52	1.43
1	D	46	TRP	CD2-CE2	5.13	1.47	1.41
1	B	76	TRP	CD2-CE2	5.06	1.47	1.41
1	D	304	TRP	CD2-CE2	5.04	1.47	1.41
1	A	235	TRP	CD2-CE2	5.02	1.47	1.41
1	A	140	PHE	CG-CD1	5.01	1.46	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	190	LYS	CD-CE-NZ	-10.54	87.45	111.70
1	A	131	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	B	145	ASP	CB-CG-OD1	7.60	125.14	118.30
1	A	131	ASP	CB-CG-OD1	6.73	124.36	118.30
1	C	131	ASP	CB-CG-OD1	6.69	124.32	118.30
1	D	145[A]	ASP	CB-CG-OD1	6.48	124.13	118.30
1	D	145[B]	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	288	LYS	CD-CE-NZ	-6.15	97.56	111.70
1	A	190[A]	LYS	CD-CE-NZ	-6.14	97.58	111.70
1	A	190[B]	LYS	CD-CE-NZ	-6.14	97.58	111.70
1	D	182	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	D	71	THR	N-CA-C	-5.77	95.42	111.00
1	B	145	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	B	131[A]	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	131[B]	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	299	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	D	94[A]	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	D	94[B]	ARG	NE-CZ-NH2	-5.45	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	THR	N-CA-C	-5.41	96.40	111.00
1	B	302	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	94[A]	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	D	94[B]	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	140	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	B	263	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	B	161	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	PHE	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	2411	0	2329	25	0
1	B	2399	0	2305	29	0
1	C	2395	0	2296	29	1
1	D	2427	0	2344	27	1
2	A	6	0	8	0	0
2	B	12	0	16	3	0
2	C	12	0	16	3	0
2	D	6	0	8	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	221	0	0	5	0
4	B	180	0	0	11	0
4	C	177	0	0	12	0
4	D	202	0	0	8	0
All	All	10456	0	9322	111	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 6.

All (111) 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:C:402:GOL:H12	4:C:543:HOH:O	1.24	1.24
1:D:202[C]:MET:SD	4:D:670:HOH:O	2.02	1.17
1:B:133:GLY:O	4:B:501:HOH:O	1.72	1.07
1:A:150:VAL:O	1:A:190[B]:LYS:HD3	1.59	1.01
1:A:133:GLY:O	4:A:501:HOH:O	1.77	1.01
1:A:280:GLU:OE1	4:A:502:HOH:O	1.79	1.01
1:D:305[A]:GLU:CG	4:D:632:HOH:O	2.14	0.95
1:D:305[A]:GLU:HG3	4:D:632:HOH:O	1.67	0.93
1:C:46:TRP:HD1	4:C:629:HOH:O	1.52	0.90
1:A:174:HIS:HE1	4:A:512:HOH:O	1.55	0.89
1:C:43[B]:THR:HG23	1:C:305[B]:GLU:HB3	1.61	0.82
1:B:80[B]:LYS:HG3	4:B:565:HOH:O	1.84	0.78
1:C:119:THR:HG23	4:C:607:HOH:O	1.83	0.76
1:C:46:TRP:CD1	4:C:629:HOH:O	2.30	0.75
1:C:98:ASN:CG	4:C:503:HOH:O	2.27	0.72
1:A:249:TYR:O	4:A:503:HOH:O	2.07	0.71
1:D:305[A]:GLU:HG2	4:D:632:HOH:O	1.83	0.71
1:C:45:LYS:HD3	1:C:305[B]:GLU:HB2	1.73	0.71
1:B:219:LYS:HE2	4:B:632:HOH:O	1.92	0.69
1:A:63:ILE:HG12	1:A:115[A]:TYR:CE1	2.27	0.69
1:A:152:ASN:HA	1:A:190[A]:LYS:HG2	1.74	0.69
1:B:131[A]:ASP:OD1	4:B:502:HOH:O	2.11	0.69
1:A:63:ILE:HG12	1:A:115[A]:TYR:CZ	2.28	0.68
1:C:63:ILE:HG12	1:C:115[A]:TYR:CZ	2.29	0.68
1:C:43[A]:THR:OG1	1:C:307:SER:OG	2.11	0.68
1:A:269:PHE:CZ	1:A:272:ASN:HA	2.31	0.66
1:B:252:ARG:HG2	1:B:252:ARG:HH11	1.61	0.65
1:B:264[B]:LYS:HG2	1:B:267:VAL:O	1.97	0.63
1:C:37:ASN:HB3	1:C:40:ASP:OD2	1.98	0.63
1:C:63:ILE:HG12	1:C:115[A]:TYR:CE1	2.35	0.62
1:C:119:THR:CG2	4:C:607:HOH:O	2.46	0.62
1:B:264[A]:LYS:HD3	4:B:661:HOH:O	1.99	0.61
1:C:119:THR:HB	4:C:506:HOH:O	2.02	0.60
1:C:145[A]:ASP:OD1	1:C:252:ARG:NH2	2.37	0.58
1:C:189[A]:VAL:HG22	1:C:198:LYS:HE2	1.86	0.58
1:A:150:VAL:O	1:A:190[A]:LYS:HD2	2.03	0.57
1:D:150:VAL:O	1:D:190:LYS:HD3	2.05	0.56
1:B:204:PRO:HD2	2:B:404:GOL:H2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:PHE:CE1	1:B:272:ASN:HA	2.41	0.56
1:C:268:LYS:HD3	1:C:269:PHE:H	1.71	0.55
1:D:63:ILE:HA	1:D:115[A]:TYR:CE2	2.42	0.54
1:D:82:VAL:HG22	1:D:91[B]:LEU:CD2	2.38	0.54
1:A:99:ASN:ND2	1:A:280:GLU:HG2	2.22	0.54
1:C:268:LYS:HD3	1:C:269:PHE:N	2.23	0.54
1:B:191:GLU:HA	4:B:515:HOH:O	2.08	0.54
1:A:268:LYS:HB2	1:A:277:ILE:HD11	1.89	0.53
1:D:63:ILE:HG12	1:D:115[A]:TYR:CZ	2.43	0.53
1:B:91[B]:LEU:HD21	1:B:112:PHE:CE2	2.44	0.53
1:B:63:ILE:HG12	1:B:115[A]:TYR:CE1	2.45	0.52
1:D:94[B]:ARG:NH1	4:D:506:HOH:O	2.38	0.52
1:D:268:LYS:HD3	1:D:269:PHE:H	1.75	0.51
1:C:63:ILE:HA	1:C:115[A]:TYR:CE2	2.45	0.51
1:B:271:ASP:N	1:B:271:ASP:OD1	2.42	0.51
1:B:83:LYS:HE2	4:B:624:HOH:O	2.11	0.50
2:C:402:GOL:C1	4:C:543:HOH:O	2.06	0.50
1:D:63:ILE:HG12	1:D:115[A]:TYR:CE1	2.47	0.49
1:B:63:ILE:HG12	1:B:115[A]:TYR:CZ	2.49	0.48
1:C:268:LYS:HB2	1:C:277:ILE:HD11	1.95	0.48
1:A:199[A]:ARG:HB2	1:A:202[A]:MET:HG3	1.94	0.47
1:B:206[B]:GLU:OE1	2:B:404:GOL:C3	2.63	0.47
1:A:148:TYR:O	1:A:190[B]:LYS:HE2	2.14	0.47
1:C:98:ASN:CB	4:C:503:HOH:O	2.63	0.47
1:C:98:ASN:HB3	4:C:503:HOH:O	2.14	0.47
1:D:72:SER:OG	1:D:273[B]:LYS:HE3	2.15	0.46
1:D:264[B]:LYS:HE2	1:D:268:LYS:HE2	1.97	0.46
1:B:119[A]:THR:HG23	4:B:513:HOH:O	2.14	0.46
1:B:203:TYR:HA	2:B:404:GOL:H2	1.97	0.46
1:B:63:ILE:HA	1:B:115[A]:TYR:CE2	2.50	0.46
1:D:177:ASP:HB2	4:D:645:HOH:O	2.15	0.46
1:B:286:ARG:NE	4:B:503:HOH:O	2.15	0.46
1:D:155:THR:HG22	1:D:252:ARG:HD3	1.98	0.46
1:B:219:LYS:CE	4:B:632:HOH:O	2.59	0.45
1:D:82:VAL:HG22	1:D:91[B]:LEU:HD23	1.97	0.45
1:D:273[B]:LYS:HD2	1:D:274[B]:ASN:H	1.80	0.45
1:A:37:ASN:OD1	1:A:39[B]:ASN:HB2	2.16	0.45
1:D:268:LYS:HD3	1:D:268:LYS:HA	1.69	0.44
1:A:170:TRP:CZ2	1:A:173:GLY:HA2	2.52	0.44
1:D:145[A]:ASP:OD1	1:D:252:ARG:NH2	2.51	0.44
1:A:158[B]:SER:HG	1:A:250:TRP:HD1	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LYS:HD2	1:B:223[B]:ILE:HD11	1.99	0.44
1:A:63:ILE:HA	1:A:115[A]:TYR:CE2	2.53	0.44
1:A:159:GLU:HB3	1:A:186:HIS:HB2	2.00	0.44
1:D:55:ASN:O	1:D:57:PRO:HD3	2.18	0.43
1:C:71:THR:HG22	4:C:648:HOH:O	2.18	0.43
1:C:67:ASN:HB3	4:C:634:HOH:O	2.17	0.43
1:A:205:GLN:NE2	1:C:192:ASN:O	2.52	0.42
1:B:184:ASN:HB3	1:B:200:PRO:HG3	2.01	0.42
1:C:279:PRO:HB2	1:C:289:LEU:HD11	2.00	0.42
1:D:54:LYS:H	1:D:54:LYS:HG2	1.51	0.42
1:B:82:VAL:HG22	1:B:91[B]:LEU:HD22	2.01	0.42
1:D:286:ARG:NE	4:D:503:HOH:O	2.32	0.42
1:D:288:LYS:HG3	4:D:520:HOH:O	2.19	0.42
1:A:150:VAL:O	1:A:190[B]:LYS:CD	2.47	0.42
1:A:271:ASP:OD1	1:A:271:ASP:N	2.51	0.42
1:B:37:ASN:HA	1:B:38:PRO:HD2	1.92	0.42
1:C:209:ASN:OD1	1:C:245:LYS:HE2	2.20	0.42
1:A:155:THR:HG22	1:A:252[A]:ARG:HD3	2.02	0.42
1:B:119[B]:THR:HB	4:B:513:HOH:O	2.19	0.42
1:C:63:ILE:HD12	1:C:113:LYS:HE2	2.02	0.41
1:C:203:TYR:HD1	2:C:402:GOL:H2	1.86	0.41
1:B:199[A]:ARG:NH2	1:B:272:ASN:HB3	2.35	0.41
1:B:133:GLY:HA2	1:B:178:ILE:CD1	2.51	0.41
1:A:275:ASN:N	1:A:275:ASN:HD22	2.19	0.41
1:C:80:LYS:HD3	1:C:80:LYS:HA	1.90	0.41
1:C:43[B]:THR:HG22	1:C:307:SER:OG	2.21	0.41
1:B:252:ARG:HH11	1:B:252:ARG:CG	2.27	0.40
1:A:55[B]:ASN:ND2	4:A:504:HOH:O	2.22	0.40
1:D:271:ASP:OD1	1:D:271:ASP:N	2.53	0.40
1:D:72:SER:OG	1:D:273[B]:LYS:HG2	2.22	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)
1:C:98:ASN:ND2	1:D:154:GLU:OE1[1_546]	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	296/286 (104%)	290 (98%)	6 (2%)	0	100	100
1	B	294/286 (103%)	286 (97%)	8 (3%)	0	100	100
1	C	293/286 (102%)	283 (97%)	10 (3%)	0	100	100
1	D	297/286 (104%)	289 (97%)	8 (3%)	0	100	100
All	All	1180/1144 (103%)	1148 (97%)	32 (3%)	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	268/255 (105%)	262 (98%)	6 (2%)	52	27
1	B	266/255 (104%)	255 (96%)	11 (4%)	30	8
1	C	265/255 (104%)	258 (97%)	7 (3%)	46	21
1	D	269/255 (106%)	261 (97%)	8 (3%)	41	15
All	All	1068/1020 (105%)	1036 (97%)	32 (3%)	43	15

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	190[A]	LYS

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Mol	Chain	Res	Type
1	A	190[B]	LYS
1	A	215	TRP
1	A	264	LYS
1	A	271	ASP
1	B	167	GLN
1	B	178	ILE
1	B	215	TRP
1	B	264[A]	LYS
1	B	264[B]	LYS
1	B	268	LYS
1	B	270	PHE
1	B	271	ASP
1	B	273	LYS
1	B	284	LYS
1	B	287	GLU
1	C	43[A]	THR
1	C	43[B]	THR
1	C	44	ILE
1	C	54	LYS
1	C	183	LEU
1	C	268	LYS
1	C	286	ARG
1	D	54	LYS
1	D	72	SER
1	D	183	LEU
1	D	190	LYS
1	D	202[B]	MET
1	D	202[C]	MET
1	D	268	LYS
1	D	271	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	275	ASN

### 5.3.3 RNA

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	D	401	-	5,5,5	0.99	0	5,5,5	0.74	0
2	GOL	B	401	-	5,5,5	0.86	0	5,5,5	0.99	0
2	GOL	B	404	-	5,5,5	0.25	0	5,5,5	1.51	1 (20%)
2	GOL	C	402	-	5,5,5	0.54	0	5,5,5	1.03	0
2	GOL	C	401	-	5,5,5	1.20	0	5,5,5	1.06	0
2	GOL	A	401	-	5,5,5	0.78	0	5,5,5	1.34	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	D	401	-	-	0/4/4/4	-
2	GOL	B	401	-	-	0/4/4/4	-
2	GOL	B	404	-	-	2/4/4/4	-
2	GOL	C	402	-	-	4/4/4/4	-
2	GOL	C	401	-	-	0/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	404	GOL	O3-C3-C2	-2.48	98.30	110.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	404	GOL	O1-C1-C2-C3
2	C	402	GOL	O1-C1-C2-C3
2	C	402	GOL	C1-C2-C3-O3
2	C	402	GOL	O2-C2-C3-O3
2	B	404	GOL	O1-C1-C2-O2
2	C	402	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	404	GOL	3	0
2	C	402	GOL	3	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 [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, 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	278/286 (97%)	-0.34	4 (1%) 75 79	16, 23, 43, 85	0
1	B	278/286 (97%)	-0.28	8 (2%) 51 52	18, 27, 50, 79	0
1	C	278/286 (97%)	-0.21	7 (2%) 57 58	17, 28, 51, 72	0
1	D	278/286 (97%)	-0.34	4 (1%) 75 79	17, 25, 45, 65	0
All	All	1112/1144 (97%)	-0.29	23 (2%) 63 65	16, 26, 49, 85	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	272	ASN	7.9
1	A	270	PHE	4.3
1	B	270	PHE	4.2
1	C	272	ASN	3.6
1	B	70[A]	ASN	3.6
1	B	272	ASN	3.6
1	A	70	ASN	3.5
1	C	46	TRP	3.4
1	B	269	PHE	3.1
1	C	277	ILE	2.9
1	B	268	LYS	2.9
1	D	273[A]	LYS	2.9
1	B	192	ASN	2.8
1	C	269	PHE	2.5
1	C	270	PHE	2.5
1	D	274[A]	ASN	2.3
1	A	269	PHE	2.3
1	D	270	PHE	2.2
1	C	119	THR	2.2
1	C	72	SER	2.1
1	B	193	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	55	ASN	2.1
1	B	72	SER	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 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, 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
2	GOL	C	402	6/6	0.89	0.20	32,43,45,46	0
2	GOL	B	404	6/6	0.93	0.20	38,44,46,50	0
2	GOL	C	401	6/6	0.95	0.09	17,21,23,28	0
2	GOL	B	401	6/6	0.97	0.07	22,25,25,27	0
2	GOL	A	401	6/6	0.97	0.09	22,23,28,32	0
3	MG	D	403	1/1	0.97	0.08	35,35,35,35	0
3	MG	B	403	1/1	0.98	0.11	41,41,41,41	0
3	MG	B	402	1/1	0.99	0.07	22,22,22,22	0
2	GOL	D	401	6/6	0.99	0.04	19,22,23,32	0
3	MG	C	404	1/1	0.99	0.06	27,27,27,27	0
3	MG	D	402	1/1	0.99	0.05	20,20,20,20	0
3	MG	A	403	1/1	0.99	0.05	32,32,32,32	0
3	MG	C	403	1/1	1.00	0.05	17,17,17,17	0
3	MG	A	402	1/1	1.00	0.05	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.