



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:41 PM UTC

PDB ID : 8A2N / pdb\_00008a2n  
Title : Structure of crocagin biosynthetic protein CgnD  
Authors : Adam, S.; Koehnke, J.  
Deposited on : 2022-06-06  
Resolution : 2.35 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

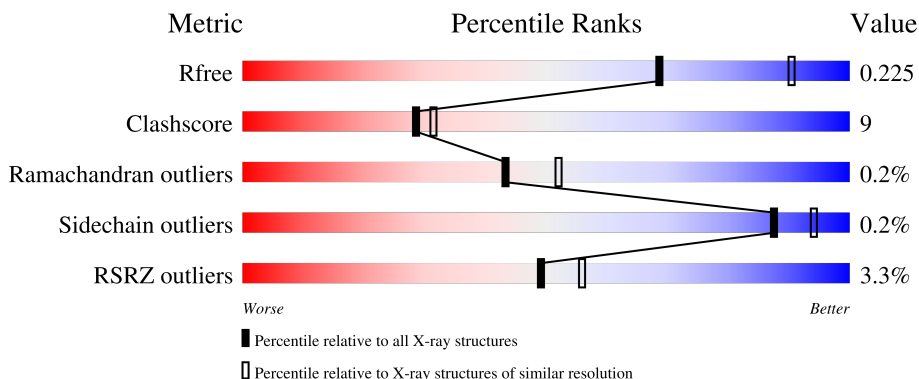
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	348	 4% 65% 18% 14%
1	B	348	 2% 73% 11% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	401	-	-	X	-
2	SO4	B	401	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9880 atoms, of which 4783 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.

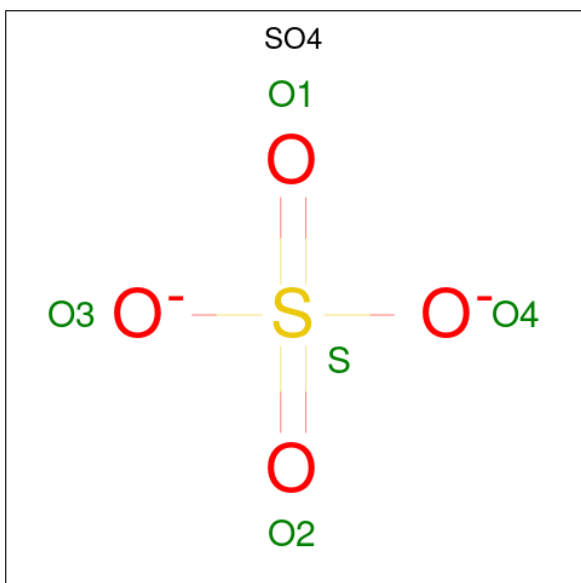
- Molecule 1 is a protein called CgnD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	B	299	4799	1545	2388	417	442	7	0	1	0
1	A	299	4820	1554	2395	424	441	6	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP A0A0K1EC25
B	0	ALA	-	expression tag	UNP A0A0K1EC25
B	?	-	SER	deletion	UNP A0A0K1EC25
A	-1	GLY	-	expression tag	UNP A0A0K1EC25
A	0	ALA	-	expression tag	UNP A0A0K1EC25
A	?	-	SER	deletion	UNP A0A0K1EC25

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

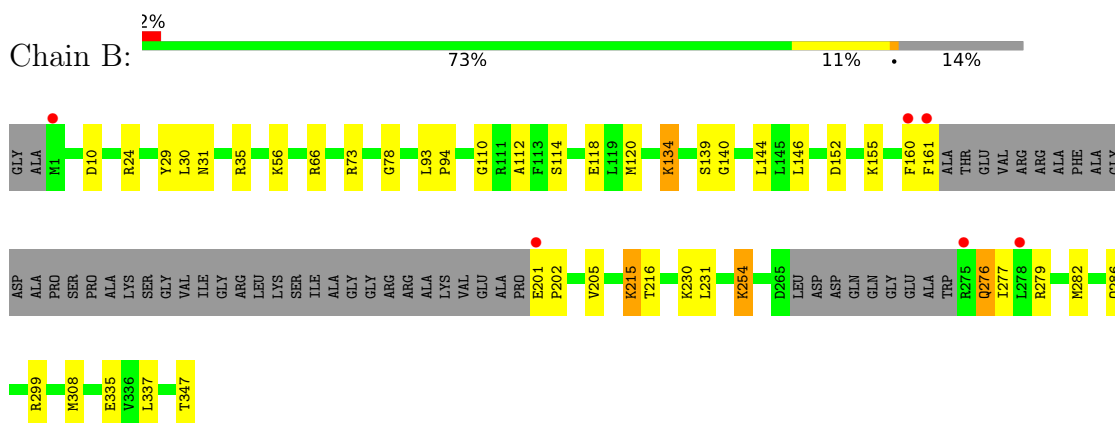
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	142	Total	O	0	0
			142	142		
3	A	109	Total	O	0	0
			109	109		

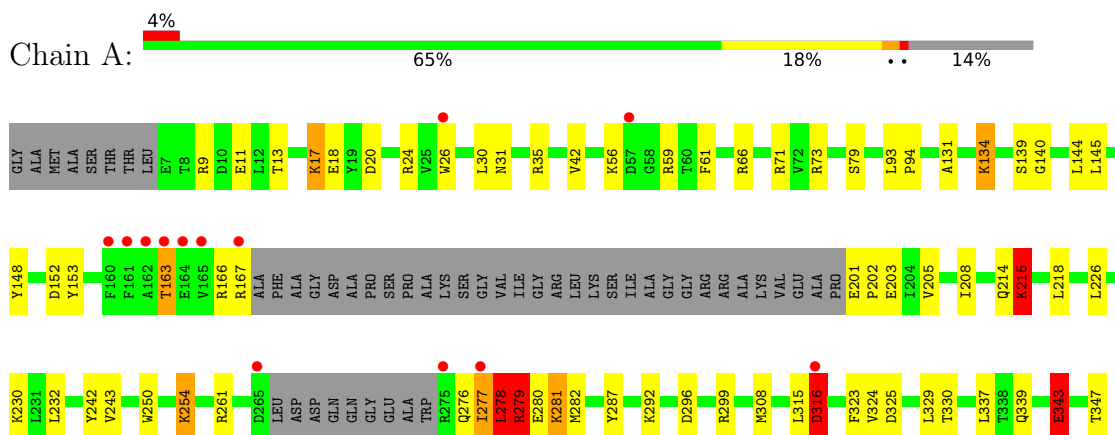
### 3 Residue-property plots [i](#)

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: CgnD



- Molecule 1: CgnD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.48Å 102.06Å 150.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 2.35 39.56 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.56-2.35) 99.7 (39.56-2.35)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.87 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.172 , 0.224 0.172 , 0.225	Depositor DCC
$R_{free}$ test set	1576 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtrriage
Anisotropy	0.365	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9880	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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: SO4, MLY

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	0.75	8/2385 (0.3%)	1.00	24/3240 (0.7%)
1	B	0.57	0/2369	0.56	1/3218 (0.0%)
All	All	0.67	8/4754 (0.2%)	0.81	25/6458 (0.4%)

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	8
1	B	0	2
All	All	0	10

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	ARG	CB-CG	14.23	1.95	1.52
1	A	316	ASP	CA-C	7.85	1.63	1.53
1	A	279	ARG	CZ-NH1	-7.38	1.22	1.32
1	A	343	GLU	CD-OE2	6.54	1.37	1.25
1	A	278	LEU	C-N	-6.52	1.24	1.33
1	A	279	ARG	CA-C	-6.33	1.44	1.52
1	A	343	GLU	CD-OE1	5.87	1.36	1.25
1	A	279	ARG	CZ-NH2	5.65	1.40	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ARG	CD-NE-CZ	24.84	159.17	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ARG	N-CA-CB	12.84	132.18	110.49
1	A	279	ARG	CB-CA-C	-12.07	86.39	110.42
1	A	279	ARG	NE-CZ-NH2	-11.99	108.41	119.20
1	A	279	ARG	CB-CG-CD	-10.28	87.67	111.30
1	A	277	ILE	N-CA-CB	9.41	122.62	110.57
1	A	343	GLU	CG-CD-OE2	-8.96	97.79	118.40
1	A	343	GLU	OE1-CD-OE2	-8.04	103.60	122.90
1	A	343	GLU	CB-CG-CD	8.02	126.23	112.60
1	A	316	ASP	CB-CA-C	-7.96	97.53	111.22
1	A	278	LEU	CA-C-N	7.85	136.53	121.54
1	A	278	LEU	C-N-CA	7.85	136.53	121.54
1	A	277	ILE	CB-CA-C	-7.00	102.85	112.02
1	A	316	ASP	OD1-CG-OD2	-6.50	107.29	122.90
1	A	343	GLU	N-CA-C	6.06	118.68	111.71
1	A	343	GLU	N-CA-CB	-6.03	100.94	110.22
1	A	343	GLU	CB-CA-C	5.81	121.38	110.63
1	A	279	ARG	N-CA-C	5.75	123.05	110.80
1	B	276	GLN	CB-CG-CD	-5.64	103.02	112.60
1	A	254	MLY	O-C-N	-5.50	114.20	123.00
1	A	276	GLN	CA-C-N	-5.25	113.83	120.56
1	A	276	GLN	C-N-CA	-5.25	113.83	120.56
1	A	277	ILE	CB-CG1-CD1	-5.19	102.91	113.80
1	A	315	LEU	CA-C-N	-5.17	115.48	123.14
1	A	315	LEU	C-N-CA	-5.17	115.48	123.14

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	MLY	Mainchain
1	A	163	THR	Peptide
1	A	17	MLY	Mainchain
1	A	215	MLY	Mainchain
1	A	254	MLY	Mainchain
1	A	278	LEU	Peptide
1	A	316	ASP	Sidechain
1	A	343	GLU	Sidechain
1	B	134	MLY	Mainchain
1	B	230	MLY	Mainchain

## 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	2425	2395	2396	54	2
1	B	2411	2388	2391	33	0
2	A	5	0	0	2	0
2	B	5	0	0	2	0
3	A	109	0	0	6	1
3	B	142	0	0	9	0
All	All	5097	4783	4787	85	3

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 9.

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:279:ARG:CG	1:A:279:ARG:CB	1.95	1.44
1:A:277:ILE:HG13	1:A:278:LEU:N	1.73	1.02
1:A:279:ARG:CB	1:A:279:ARG:CD	2.43	0.96
1:B:299:ARG:NH1	3:B:502:HOH:O	1.93	0.86
2:B:401:SO4:O4	3:B:501:HOH:O	1.93	0.85
1:A:11:GLU:OE2	3:A:501:HOH:O	1.93	0.85
1:A:66:ARG:NH2	3:A:502:HOH:O	2.05	0.76
1:B:308:MET:HG2	1:B:337:LEU:HD11	1.71	0.73
1:B:146[B]:LEU:HD21	1:B:161:PHE:CG	2.23	0.73
1:A:203:GLU:OE1	3:A:503:HOH:O	2.06	0.73
1:A:73:ARG:NH1	1:A:347:THR:O	2.22	0.72
1:A:279:ARG:CB	1:A:279:ARG:HD3	2.19	0.71
1:B:347:THR:OXT	3:B:503:HOH:O	2.09	0.70
1:A:277:ILE:HG13	1:A:278:LEU:H	1.57	0.67
1:A:339:GLN:NE2	1:A:343:GLU:OE1	2.28	0.67
1:A:11:GLU:CD	3:A:501:HOH:O	2.37	0.65
1:A:152:ASP:HB3	1:A:205:VAL:HG12	1.81	0.63
1:B:146[B]:LEU:HD21	1:B:161:PHE:CD2	2.34	0.61
1:B:202:PRO:O	1:A:35:ARG:NH1	2.34	0.60
1:A:279:ARG:CG	1:A:279:ARG:CA	2.80	0.59
1:B:24:ARG:NH2	2:B:401:SO4:O1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:MLY:HG3	1:A:56:MLY:HH13	1.84	0.58
1:B:215:MLY:HH12	1:B:286:GLN:OE1	2.03	0.58
1:A:139:SER:OG	1:A:140:GLY:N	2.37	0.58
1:B:335:GLU:OE1	3:B:505:HOH:O	2.18	0.57
1:B:201:GLU:HG3	1:A:35:ARG:HD3	1.87	0.57
1:B:10:ASP:OD1	3:B:504:HOH:O	2.17	0.57
1:A:339:GLN:O	1:A:343:GLU:HB2	2.05	0.57
1:B:152:ASP:HB3	1:B:205:VAL:HG12	1.86	0.57
1:A:280:GLU:HA	1:A:280:GLU:OE1	2.05	0.56
1:B:231:LEU:HD21	1:A:232:LEU:HD23	1.87	0.56
1:B:276:GLN:O	1:B:279:ARG:N	2.39	0.55
1:B:146[B]:LEU:HD13	1:B:160:PHE:HA	1.89	0.55
1:B:35:ARG:HD2	3:B:538:HOH:O	2.07	0.54
1:A:324:VAL:HG12	1:A:330:THR:HG22	1.90	0.54
1:A:79:SER:OG	2:A:401:SO4:O3	2.21	0.53
1:B:146[B]:LEU:HD21	1:B:161:PHE:CD1	2.44	0.53
1:A:9:ARG:NH2	1:A:20:ASP:OD2	2.37	0.52
1:B:144:LEU:HG	1:B:282:MET:HE1	1.94	0.49
1:B:276:GLN:O	1:B:277:ILE:C	2.55	0.49
1:A:201:GLU:N	3:A:514:HOH:O	2.45	0.49
1:A:144:LEU:CD2	1:A:282:MET:HE1	2.43	0.49
1:B:112:ALA:HB1	1:B:161:PHE:CD2	2.48	0.49
1:A:18:GLU:HG2	1:A:42:VAL:HB	1.95	0.48
1:A:30:LEU:O	1:A:31:ASN:HB2	2.14	0.48
1:B:216:THR:HG23	3:B:555:HOH:O	2.12	0.48
1:A:166:ARG:O	1:A:167:ARG:HB3	2.14	0.48
1:A:148:TYR:CD2	1:A:281:MLY:HG3	2.49	0.47
1:B:66:ARG:NH2	3:B:516:HOH:O	2.46	0.47
1:B:114:SER:O	1:B:118:GLU:HG3	2.15	0.46
1:A:296:ASP:OD1	1:A:299:ARG:NH2	2.49	0.46
1:B:308:MET:CG	1:B:337:LEU:HD11	2.43	0.46
1:A:59:ARG:HD3	1:A:61:PHE:CZ	2.51	0.46
1:A:250:TRP:CZ2	1:A:282:MET:HE3	2.51	0.46
1:A:24:ARG:NH2	2:A:401:SO4:O4	2.49	0.44
1:A:243:VAL:CG1	1:A:308:MET:HG2	2.48	0.44
1:A:329:LEU:HD11	1:A:337:LEU:HD12	1.99	0.43
1:B:29:TYR:HB3	1:B:120:MET:HE1	2.00	0.43
1:A:167:ARG:N	1:A:167:ARG:HD3	2.32	0.43
1:B:139:SER:OG	1:B:140:GLY:N	2.46	0.43
1:A:13:THR:HG21	1:A:324:VAL:HB	2.00	0.43
1:A:163:THR:HG22	1:A:163:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:HD22	1:A:277:ILE:HD11	2.01	0.43
1:B:30:LEU:O	1:B:31:ASN:HB2	2.19	0.42
1:A:93:LEU:HB2	1:A:94:PRO:HD3	2.01	0.42
1:B:93:LEU:HB2	1:B:94:PRO:HD3	2.01	0.42
1:B:73:ARG:NH1	1:B:347:THR:OXT	2.51	0.42
1:A:308:MET:HE2	1:A:337:LEU:HG	2.01	0.42
1:A:26[B]:TRP:HE3	1:A:31:ASN:O	2.03	0.42
1:B:93:LEU:HD11	1:B:337:LEU:HD23	2.01	0.42
1:B:254:MLY:HD2	1:B:254:MLY:HH23	1.83	0.42
1:A:153:TYR:HB2	1:A:208:ILE:HD11	2.02	0.42
1:A:66:ARG:NH1	1:A:131:ALA:O	2.50	0.41
1:A:201:GLU:N	1:A:202:PRO:CD	2.83	0.41
1:A:250:TRP:CE2	1:A:287:TYR:HB2	2.55	0.41
1:A:214:GLN:O	1:A:215:MLY:C	2.69	0.41
1:A:218:LEU:C	1:A:218:LEU:HD12	2.46	0.41
1:A:226:LEU:HD21	1:A:242:TYR:CD1	2.56	0.41
1:B:161:PHE:HA	3:B:514:HOH:O	2.21	0.41
1:A:323:PHE:HB3	1:A:325:ASP:O	2.21	0.41
1:A:324:VAL:CG1	1:A:330:THR:HG22	2.51	0.41
1:B:78:GLY:HA2	1:B:110:GLY:O	2.21	0.41
1:A:261:ARG:NH1	3:A:501:HOH:O	2.25	0.40
1:A:24:ARG:HG3	1:A:24:ARG:NH1	2.36	0.40
1:A:250:TRP:HZ2	1:A:282:MET:HE3	1.87	0.40

All (3) 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:A:71:ARG:NH1	1:A:316:ASP:OD1[4_467]	1.66	0.54
1:A:71:ARG:HH11	1:A:316:ASP:OD1[4_467]	1.19	0.41
3:A:573:HOH:O	3:A:600:HOH:O[4_567]	1.93	0.27

## 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	285/348 (82%)	271 (95%)	13 (5%)	1 (0%)	30	34
1	B	285/348 (82%)	275 (96%)	10 (4%)	0	100	100
All	All	570/696 (82%)	546 (96%)	23 (4%)	1 (0%)	43	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	ARG

### 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	246/277 (89%)	245 (100%)	1 (0%)	84	91
1	B	246/277 (89%)	246 (100%)	0	100	100
All	All	492/554 (89%)	491 (100%)	1 (0%)	87	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	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](#)

18 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	B	281	1	9,10,11	1.11	0	6,11,13	1.00	0
1	MLY	B	215	1	9,10,11	1.16	1 (11%)	6,11,13	0.97	0
1	MLY	B	155	1	9,10,11	0.83	0	6,11,13	1.20	1 (16%)
1	MLY	B	230	1	9,10,11	1.02	0	6,11,13	1.25	0
1	MLY	B	254	1	9,10,11	1.13	1 (11%)	6,11,13	1.12	0
1	MLY	A	17	1	9,10,11	0.76	0	6,11,13	1.68	1 (16%)
1	MLY	A	134	1	9,10,11	0.88	0	6,11,13	1.37	1 (16%)
1	MLY	A	281	1	9,10,11	1.25	1 (11%)	6,11,13	1.42	2 (33%)
1	MLY	A	230	1	9,10,11	1.28	1 (11%)	6,11,13	1.24	1 (16%)
1	MLY	A	292	1	9,10,11	1.15	0	6,11,13	1.39	1 (16%)
1	MLY	A	155	1	9,10,11	0.60	0	6,11,13	1.20	0
1	MLY	A	254	1	9,10,11	0.93	0	6,11,13	0.96	0
1	MLY	B	17	1	9,10,11	0.86	0	6,11,13	1.22	0
1	MLY	B	134	1	9,10,11	0.70	0	6,11,13	1.49	1 (16%)
1	MLY	B	56	1	9,10,11	0.72	0	6,11,13	2.10	1 (16%)
1	MLY	B	292	1	9,10,11	0.90	0	6,11,13	0.98	0
1	MLY	A	215	1	9,10,11	0.98	0	6,11,13	1.32	1 (16%)
1	MLY	A	56	1	9,10,11	0.78	0	6,11,13	1.02	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
1	MLY	B	281	1	-	0/8/9/11	-
1	MLY	B	215	1	-	5/8/9/11	-
1	MLY	B	155	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	230	1	-	3/8/9/11	-
1	MLY	B	254	1	-	2/8/9/11	-
1	MLY	A	17	1	-	3/8/9/11	-
1	MLY	A	134	1	-	0/8/9/11	-
1	MLY	A	281	1	-	4/8/9/11	-
1	MLY	A	230	1	-	3/8/9/11	-
1	MLY	A	292	1	-	5/8/9/11	-
1	MLY	A	155	1	-	2/8/9/11	-
1	MLY	A	254	1	-	2/8/9/11	-
1	MLY	B	17	1	-	5/8/9/11	-
1	MLY	B	134	1	-	1/8/9/11	-
1	MLY	B	56	1	-	5/8/9/11	-
1	MLY	B	292	1	-	2/8/9/11	-
1	MLY	A	215	1	-	3/8/9/11	-
1	MLY	A	56	1	-	1/8/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	MLY	CB-CA	-2.79	1.49	1.53
1	B	215	MLY	CD-CE	-2.40	1.42	1.51
1	A	281	MLY	CB-CA	-2.25	1.50	1.53
1	B	254	MLY	CB-CA	-2.15	1.50	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	MLY	CD-CE-NZ	4.81	126.13	113.71
1	A	17	MLY	CD-CE-NZ	2.98	121.42	113.71
1	A	134	MLY	CD-CE-NZ	2.91	121.23	113.71
1	A	230	MLY	CD-CG-CB	2.66	123.64	113.62
1	A	292	MLY	CD-CE-NZ	2.36	119.80	113.71
1	B	134	MLY	CD-CE-NZ	2.32	119.71	113.71
1	A	215	MLY	CG-CD-CE	2.24	123.33	113.17
1	B	155	MLY	CG-CD-CE	2.22	123.27	113.17
1	A	281	MLY	CH2-NZ-CE	-2.22	101.95	110.75
1	A	281	MLY	CD-CG-CB	2.19	121.88	113.62

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	56	MLY	C-CA-CB-CG
1	B	215	MLY	N-CA-CB-CG
1	B	215	MLY	C-CA-CB-CG
1	B	230	MLY	N-CA-CB-CG
1	B	230	MLY	C-CA-CB-CG
1	A	215	MLY	C-CA-CB-CG
1	A	281	MLY	C-CA-CB-CG
1	A	292	MLY	C-CA-CB-CG
1	A	254	MLY	CG-CD-CE-NZ
1	B	17	MLY	CD-CE-NZ-CH2
1	B	155	MLY	CD-CE-NZ-CH2
1	A	155	MLY	CD-CE-NZ-CH2
1	A	281	MLY	CD-CE-NZ-CH1
1	A	281	MLY	CD-CE-NZ-CH2
1	A	292	MLY	CD-CE-NZ-CH2
1	B	155	MLY	CG-CD-CE-NZ
1	A	17	MLY	CG-CD-CE-NZ
1	B	254	MLY	CG-CD-CE-NZ
1	A	292	MLY	CG-CD-CE-NZ
1	B	215	MLY	CD-CE-NZ-CH1
1	B	56	MLY	CE-CD-CG-CB
1	A	230	MLY	CG-CD-CE-NZ
1	B	17	MLY	CD-CE-NZ-CH1
1	A	254	MLY	CE-CD-CG-CB
1	A	155	MLY	CD-CE-NZ-CH1
1	B	56	MLY	CA-CB-CG-CD
1	A	56	MLY	CA-CB-CG-CD
1	A	230	MLY	CE-CD-CG-CB
1	A	17	MLY	CE-CD-CG-CB
1	B	134	MLY	CE-CD-CG-CB
1	A	292	MLY	CE-CD-CG-CB
1	B	215	MLY	CA-CB-CG-CD
1	A	281	MLY	CG-CD-CE-NZ
1	B	230	MLY	CE-CD-CG-CB
1	B	17	MLY	CE-CD-CG-CB
1	B	292	MLY	CG-CD-CE-NZ
1	B	292	MLY	CE-CD-CG-CB
1	B	56	MLY	CD-CE-NZ-CH2
1	B	155	MLY	CA-CB-CG-CD
1	B	155	MLY	CD-CE-NZ-CH1
1	B	254	MLY	CD-CE-NZ-CH2
1	A	292	MLY	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	B	155	MLY	CE-CD-CG-CB
1	A	215	MLY	CD-CE-NZ-CH2
1	B	17	MLY	CG-CD-CE-NZ
1	B	56	MLY	CG-CD-CE-NZ
1	B	215	MLY	CD-CE-NZ-CH2
1	A	230	MLY	CA-CB-CG-CD
1	B	17	MLY	C-CA-CB-CG
1	A	17	MLY	C-CA-CB-CG
1	A	215	MLY	CA-CB-CG-CD

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	215	MLY	1	0
1	B	254	MLY	1	0
1	A	281	MLY	1	0
1	A	215	MLY	1	0
1	A	56	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	SO4	B	401	-	4,4,4	0.33	0	6,6,6	0.24	0
2	SO4	A	401	-	4,4,4	0.33	0	6,6,6	0.26	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SO4	2	0
2	A	401	SO4	2	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	290/348 (83%)	-0.11	13 (4%) 38 44	15, 36, 71, 98	1 (0%)
1	B	290/348 (83%)	-0.28	6 (2%) 63 68	18, 33, 64, 90	1 (0%)
All	All	580/696 (83%)	-0.20	19 (3%) 49 56	15, 35, 69, 98	2 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	PHE	5.9
1	A	165	VAL	5.1
1	A	161	PHE	4.7
1	A	163	THR	3.9
1	B	278	LEU	3.8
1	A	164	GLU	3.3
1	A	26[A]	TRP	3.1
1	A	167	ARG	3.1
1	B	275	ARG	2.9
1	A	277	ILE	2.7
1	A	275	ARG	2.6
1	A	162	ALA	2.3
1	A	316	ASP	2.3
1	A	160	PHE	2.3
1	A	57	ASP	2.3
1	B	201	GLU	2.3
1	B	160	PHE	2.2
1	A	265	ASP	2.2
1	B	1	MET	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
1	MLY	A	56	11/12	0.66	0.23	67,80,92,94	0
1	MLY	B	56	11/12	0.73	0.25	47,95,128,146	0
1	MLY	B	155	11/12	0.82	0.26	27,76,118,138	0
1	MLY	A	254	11/12	0.84	0.20	39,83,106,106	0
1	MLY	A	292	11/12	0.88	0.17	32,75,102,102	0
1	MLY	B	254	11/12	0.89	0.15	32,69,106,106	0
1	MLY	B	17	11/12	0.89	0.15	24,58,93,93	0
1	MLY	A	17	11/12	0.90	0.16	32,73,107,107	0
1	MLY	B	281	11/12	0.91	0.10	36,54,70,70	0
1	MLY	A	230	11/12	0.91	0.12	30,52,69,69	0
1	MLY	A	155	11/12	0.92	0.14	29,53,105,105	0
1	MLY	A	215	11/12	0.93	0.10	29,47,55,55	0
1	MLY	A	281	11/12	0.93	0.10	40,54,69,69	0
1	MLY	A	134	11/12	0.93	0.11	29,55,72,72	0
1	MLY	B	292	11/12	0.94	0.13	29,64,80,82	0
1	MLY	B	215	11/12	0.94	0.08	24,38,42,42	0
1	MLY	B	134	11/12	0.95	0.08	26,48,69,69	0
1	MLY	B	230	11/12	0.95	0.09	24,49,67,67	0

### 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
2	SO4	B	401	5/5	0.97	0.08	35,36,46,47	0
2	SO4	A	401	5/5	0.97	0.10	38,39,49,57	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.