



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 10:34 am BST

PDB ID : 8BDQ  
Title : Crystal structure of Bacteroides ovatus CP926 PL38 alginate lyase  
Authors : Roenne, M.E.; Tandrup, T.; Wilkens, C.  
Deposited on : 2022-10-19  
Resolution : 2.11 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>.

---

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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

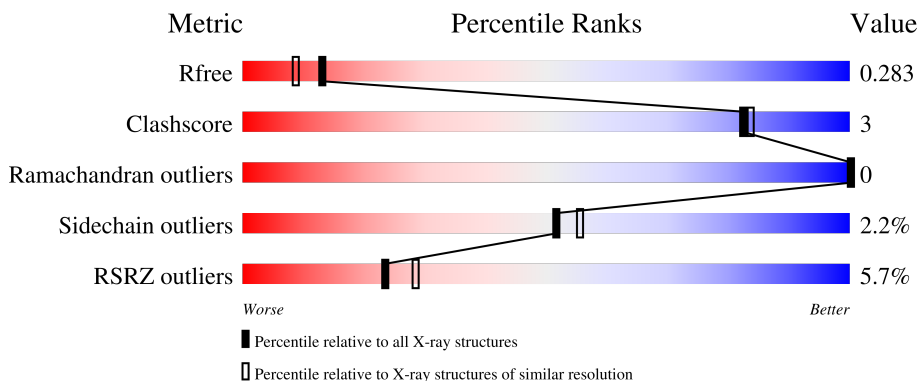
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	404	 5% 85% 8% 6%
1	B	404	 6% 86% 8% 6%
1	C	404	 5% 87% 7% 6%
1	D	404	 4% 85% 9% 6%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 12356 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 Alginate lyase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	379	Total 3055	C 1954	N 517	O 571	S 13	0	1	0
1	B	380	Total 3061	C 1957	N 518	O 573	S 13	0	1	0
1	C	380	Total 3069	C 1962	N 519	O 574	S 14	0	2	0
1	D	381	Total 3066	C 1960	N 519	O 574	S 13	0	1	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5M5BWR5
A	2	GLY	-	expression tag	UNP A0A5M5BWR5
A	3	SER	-	expression tag	UNP A0A5M5BWR5
A	4	SER	-	expression tag	UNP A0A5M5BWR5
A	5	HIS	-	expression tag	UNP A0A5M5BWR5
A	6	HIS	-	expression tag	UNP A0A5M5BWR5
A	7	HIS	-	expression tag	UNP A0A5M5BWR5
A	8	HIS	-	expression tag	UNP A0A5M5BWR5
A	9	HIS	-	expression tag	UNP A0A5M5BWR5
A	10	HIS	-	expression tag	UNP A0A5M5BWR5
A	11	SER	-	expression tag	UNP A0A5M5BWR5
A	12	SER	-	expression tag	UNP A0A5M5BWR5
A	13	GLY	-	expression tag	UNP A0A5M5BWR5
A	14	LEU	-	expression tag	UNP A0A5M5BWR5
A	15	VAL	-	expression tag	UNP A0A5M5BWR5
A	16	PRO	-	expression tag	UNP A0A5M5BWR5
A	17	ARG	-	expression tag	UNP A0A5M5BWR5
A	18	GLY	-	expression tag	UNP A0A5M5BWR5
A	19	SER	-	expression tag	UNP A0A5M5BWR5
A	20	HIS	-	expression tag	UNP A0A5M5BWR5
A	21	MET	-	expression tag	UNP A0A5M5BWR5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP A0A5M5BWR5
A	23	SER	-	expression tag	UNP A0A5M5BWR5
B	1	MET	-	initiating methionine	UNP A0A5M5BWR5
B	2	GLY	-	expression tag	UNP A0A5M5BWR5
B	3	SER	-	expression tag	UNP A0A5M5BWR5
B	4	SER	-	expression tag	UNP A0A5M5BWR5
B	5	HIS	-	expression tag	UNP A0A5M5BWR5
B	6	HIS	-	expression tag	UNP A0A5M5BWR5
B	7	HIS	-	expression tag	UNP A0A5M5BWR5
B	8	HIS	-	expression tag	UNP A0A5M5BWR5
B	9	HIS	-	expression tag	UNP A0A5M5BWR5
B	10	HIS	-	expression tag	UNP A0A5M5BWR5
B	11	SER	-	expression tag	UNP A0A5M5BWR5
B	12	SER	-	expression tag	UNP A0A5M5BWR5
B	13	GLY	-	expression tag	UNP A0A5M5BWR5
B	14	LEU	-	expression tag	UNP A0A5M5BWR5
B	15	VAL	-	expression tag	UNP A0A5M5BWR5
B	16	PRO	-	expression tag	UNP A0A5M5BWR5
B	17	ARG	-	expression tag	UNP A0A5M5BWR5
B	18	GLY	-	expression tag	UNP A0A5M5BWR5
B	19	SER	-	expression tag	UNP A0A5M5BWR5
B	20	HIS	-	expression tag	UNP A0A5M5BWR5
B	21	MET	-	expression tag	UNP A0A5M5BWR5
B	22	ALA	-	expression tag	UNP A0A5M5BWR5
B	23	SER	-	expression tag	UNP A0A5M5BWR5
C	1	MET	-	initiating methionine	UNP A0A5M5BWR5
C	2	GLY	-	expression tag	UNP A0A5M5BWR5
C	3	SER	-	expression tag	UNP A0A5M5BWR5
C	4	SER	-	expression tag	UNP A0A5M5BWR5
C	5	HIS	-	expression tag	UNP A0A5M5BWR5
C	6	HIS	-	expression tag	UNP A0A5M5BWR5
C	7	HIS	-	expression tag	UNP A0A5M5BWR5
C	8	HIS	-	expression tag	UNP A0A5M5BWR5
C	9	HIS	-	expression tag	UNP A0A5M5BWR5
C	10	HIS	-	expression tag	UNP A0A5M5BWR5
C	11	SER	-	expression tag	UNP A0A5M5BWR5
C	12	SER	-	expression tag	UNP A0A5M5BWR5
C	13	GLY	-	expression tag	UNP A0A5M5BWR5
C	14	LEU	-	expression tag	UNP A0A5M5BWR5
C	15	VAL	-	expression tag	UNP A0A5M5BWR5
C	16	PRO	-	expression tag	UNP A0A5M5BWR5
C	17	ARG	-	expression tag	UNP A0A5M5BWR5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLY	-	expression tag	UNP A0A5M5BWR5
C	19	SER	-	expression tag	UNP A0A5M5BWR5
C	20	HIS	-	expression tag	UNP A0A5M5BWR5
C	21	MET	-	expression tag	UNP A0A5M5BWR5
C	22	ALA	-	expression tag	UNP A0A5M5BWR5
C	23	SER	-	expression tag	UNP A0A5M5BWR5
D	1	MET	-	initiating methionine	UNP A0A5M5BWR5
D	2	GLY	-	expression tag	UNP A0A5M5BWR5
D	3	SER	-	expression tag	UNP A0A5M5BWR5
D	4	SER	-	expression tag	UNP A0A5M5BWR5
D	5	HIS	-	expression tag	UNP A0A5M5BWR5
D	6	HIS	-	expression tag	UNP A0A5M5BWR5
D	7	HIS	-	expression tag	UNP A0A5M5BWR5
D	8	HIS	-	expression tag	UNP A0A5M5BWR5
D	9	HIS	-	expression tag	UNP A0A5M5BWR5
D	10	HIS	-	expression tag	UNP A0A5M5BWR5
D	11	SER	-	expression tag	UNP A0A5M5BWR5
D	12	SER	-	expression tag	UNP A0A5M5BWR5
D	13	GLY	-	expression tag	UNP A0A5M5BWR5
D	14	LEU	-	expression tag	UNP A0A5M5BWR5
D	15	VAL	-	expression tag	UNP A0A5M5BWR5
D	16	PRO	-	expression tag	UNP A0A5M5BWR5
D	17	ARG	-	expression tag	UNP A0A5M5BWR5
D	18	GLY	-	expression tag	UNP A0A5M5BWR5
D	19	SER	-	expression tag	UNP A0A5M5BWR5
D	20	HIS	-	expression tag	UNP A0A5M5BWR5
D	21	MET	-	expression tag	UNP A0A5M5BWR5
D	22	ALA	-	expression tag	UNP A0A5M5BWR5
D	23	SER	-	expression tag	UNP A0A5M5BWR5

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

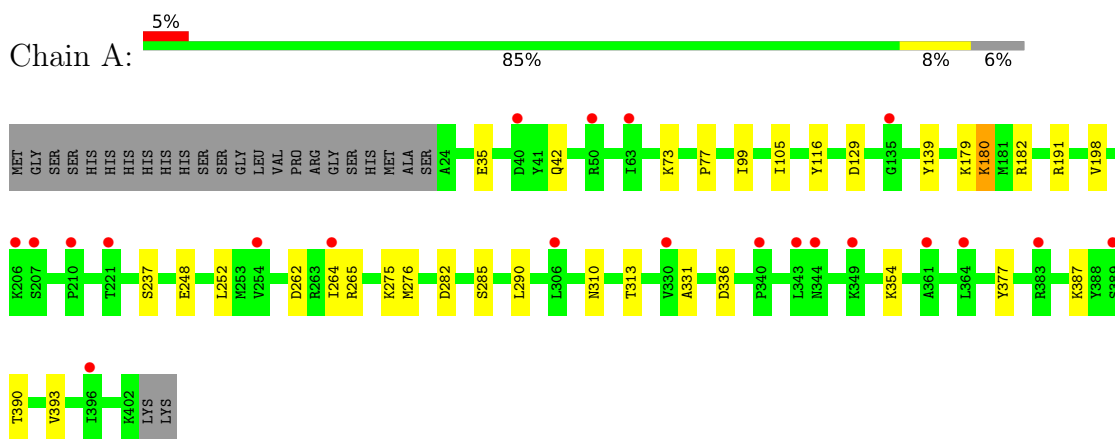
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	21	Total	O	0	0
			21	21		
3	C	21	Total	O	0	0
			21	21		
3	D	20	Total	O	0	0
			20	20		

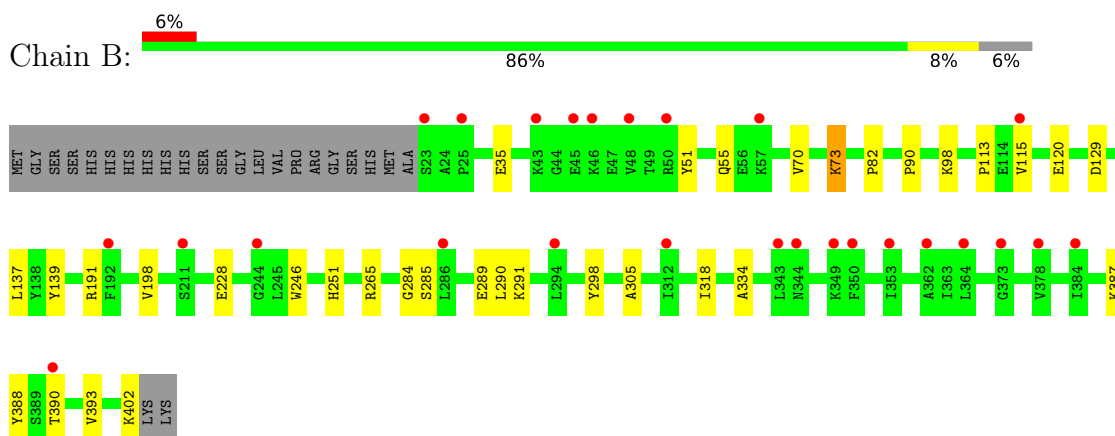
### 3 Residue-property plots [i](#)

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.

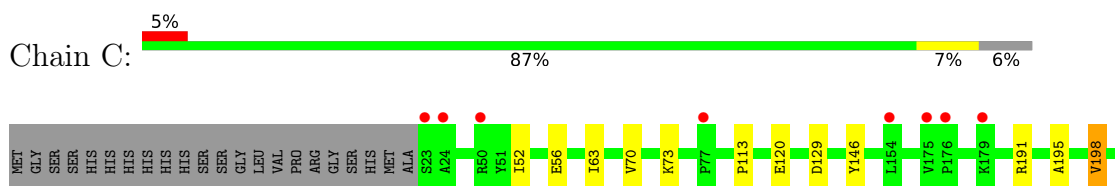
- Molecule 1: Alginate lyase family protein



- Molecule 1: Alginate lyase family protein

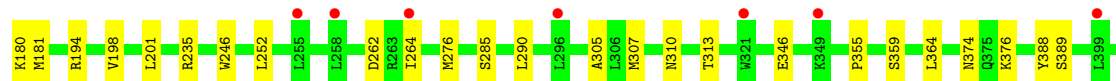
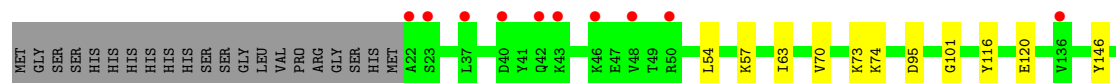
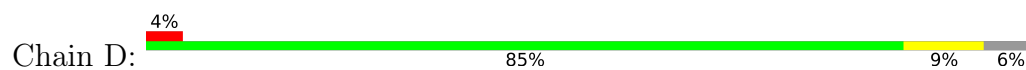


- Molecule 1: Alginate lyase family protein





- Molecule 1: Alginate lyase family protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	196.70Å 88.09Å 144.00Å 90.00° 120.06° 90.00°	Depositor
Resolution (Å)	48.12 – 2.11 49.17 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.12-2.11) 99.2 (49.17-2.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 2.12Å)	Xtrriage
Refinement program	REFMAC 8.0, PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.255 , 0.281 0.257 , 0.283	Depositor DCC
$R_{free}$ test set	2101 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtrriage
Anisotropy	0.230	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 29.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12356	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.79% 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

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	0.27	0/3133	0.47	0/4246
1	B	0.27	0/3139	0.47	0/4254
1	C	0.26	0/3147	0.47	0/4264
1	D	0.26	0/3144	0.47	0/4261
All	All	0.26	0/12563	0.47	0/17025

There are no bond length outliers.

There are no bond angle outliers.

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	3055	0	3024	15	0
1	B	3061	0	3029	18	0
1	C	3069	0	3037	14	0
1	D	3066	0	3034	18	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	18	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	0	0	0
3	C	21	0	0	1	0
3	D	20	0	0	0	0
All	All	12356	0	12124	62	0

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

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLU:OE2	1:B:139:TYR:OH	2.12	0.67
1:B:387:LYS:HB2	1:B:390:THR:HG23	1.85	0.58
1:A:336:ASP:OD1	1:A:377:TYR:OH	2.18	0.57
1:C:195:ALA:O	1:C:198:VAL:HG12	2.08	0.54
1:A:180:LYS:HE3	1:A:180:LYS:H	1.72	0.54
1:A:262:ASP:OD1	1:A:265:ARG:NH1	2.40	0.54
1:D:54:LEU:HD21	1:D:389:SER:HA	1.89	0.54
1:A:35:GLU:OE2	1:A:139:TYR:OH	2.24	0.53
1:D:285:SER:HB2	1:D:290:LEU:HD11	1.90	0.53
1:C:353:ILE:HB	1:D:355:PRO:HD3	1.89	0.53
1:B:73:LYS:NZ	1:B:120:GLU:OE2	2.38	0.52
1:D:252:LEU:HD22	1:D:264:ILE:HG23	1.92	0.51
1:C:295:SER:HG	1:C:348:TRP:HE1	1.59	0.51
1:B:70:VAL:HG23	1:B:120:GLU:HG2	1.93	0.50
1:C:70:VAL:HG23	1:C:120:GLU:HG2	1.93	0.50
1:C:279:GLN:NE2	3:C:601:H0H:O	2.35	0.49
1:B:73:LYS:HD2	1:B:82:PRO:HA	1.96	0.48
1:B:388:TYR:HA	1:B:402:LYS:HB3	1.95	0.48
1:A:276:MET:SD	1:A:331:ALA:HB2	2.53	0.48
1:B:228:GLU:OE2	1:B:251:HIS:NE2	2.44	0.47
1:A:129:ASP:HA	1:A:393:VAL:HG21	1.97	0.47
1:A:252:LEU:HD22	1:A:264:ILE:HG23	1.95	0.47
1:D:307:MET:HE2	1:D:364:LEU:HD13	1.97	0.46
1:D:181:MET:O	1:D:235:ARG:NH1	2.47	0.46
1:B:285:SER:HB2	1:B:290:LEU:HD11	1.99	0.44
1:D:70:VAL:HG23	1:D:120:GLU:HG2	2.00	0.44
1:A:73:LYS:HE3	1:A:77:PRO:HD3	1.98	0.44
1:D:63:ILE:HD11	1:D:146:TYR:CE1	2.53	0.44
1:C:353:ILE:HG13	1:C:354:LYS:HD2	2.00	0.44
1:B:246:TRP:CE2	1:B:305:ALA:HB2	2.53	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ILE:O	1:C:56:GLU:HG3	2.18	0.44
1:D:95:ASP:O	1:D:101:GLY:HA2	2.17	0.44
1:A:248:GLU:HA	1:A:248:GLU:OE1	2.17	0.44
1:A:237:SER:O	1:A:275:LYS:NZ	2.32	0.44
1:A:285:SER:HB2	1:A:290:LEU:HD11	1.99	0.43
1:A:387:LYS:HB2	1:A:390:THR:HG23	2.00	0.43
1:C:129:ASP:HA	1:C:393:VAL:HG21	1.99	0.43
1:B:129:ASP:HA	1:B:393:VAL:HG21	2.00	0.43
1:A:354:LYS:HB3	1:A:354:LYS:HE2	1.86	0.43
1:C:246:TRP:CD1	1:C:305:ALA:HB2	2.54	0.43
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.83	0.43
1:D:198:VAL:HG13	1:D:201:LEU:HD12	2.01	0.42
1:B:90:PRO:HA	1:B:115:VAL:HG11	2.01	0.42
1:B:284:GLY:O	1:B:334:ALA:HA	2.19	0.42
1:D:374:ASN:OD1	1:D:376:LYS:HG2	2.20	0.42
1:B:98:LYS:HB3	1:B:98:LYS:HE2	1.81	0.42
1:D:262:ASP:N	1:D:262:ASP:OD1	2.53	0.42
1:C:113:PRO:HB3	1:D:116:TYR:CZ	2.55	0.42
1:B:265:ARG:HG3	1:B:318:ILE:HD11	2.01	0.42
1:C:63:ILE:HD11	1:C:146:TYR:CE1	2.55	0.42
1:A:116:TYR:CZ	1:B:113:PRO:HB3	2.55	0.41
1:D:388:TYR:HA	1:D:402:LYS:HB3	2.02	0.41
1:B:51:TYR:O	1:B:55:GLN:HG2	2.20	0.41
1:D:70:VAL:CG2	1:D:120:GLU:HG2	2.51	0.41
1:D:194:ARG:O	1:D:198:VAL:HG23	2.20	0.41
1:D:246:TRP:CD1	1:D:305:ALA:HB2	2.56	0.41
1:C:388:TYR:HA	1:C:402:LYS:HB3	2.03	0.41
1:C:285:SER:HB2	1:C:290:LEU:HD11	2.03	0.40
1:A:310:ASN:HA	1:A:313:THR:OG1	2.22	0.40
1:D:310:ASN:HA	1:D:313:THR:OG1	2.21	0.40
1:B:289:GLU:OE1	1:B:298:TYR:HB3	2.22	0.40
1:C:246:TRP:CE2	1:C:305:ALA:HB2	2.57	0.40

There are no symmetry-related clashes.

## 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	378/404 (94%)	370 (98%)	8 (2%)	0	100	100
1	B	379/404 (94%)	369 (97%)	10 (3%)	0	100	100
1	C	380/404 (94%)	373 (98%)	7 (2%)	0	100	100
1	D	380/404 (94%)	373 (98%)	7 (2%)	0	100	100
All	All	1517/1616 (94%)	1485 (98%)	32 (2%)	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	324/344 (94%)	315 (97%)	9 (3%)	43	46
1	B	325/344 (94%)	321 (99%)	4 (1%)	71	77
1	C	326/344 (95%)	318 (98%)	8 (2%)	47	50
1	D	325/344 (94%)	318 (98%)	7 (2%)	52	55
All	All	1300/1376 (94%)	1272 (98%)	28 (2%)	52	55

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	99	ILE
1	A	105	ILE
1	A	179	LYS
1	A	180	LYS
1	A	182	ARG
1	A	191	ARG
1	A	198	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	282	ASP
1	B	73	LYS
1	B	191	ARG
1	B	198	VAL
1	B	291	LYS
1	C	73	LYS
1	C	191	ARG
1	C	198	VAL
1	C	235	ARG
1	C	262	ASP
1	C	359	SER
1	C	376	LYS
1	C	390	THR
1	D	57	LYS
1	D	73	LYS
1	D	74	LYS
1	D	180	LYS
1	D	276	MET
1	D	346	GLU
1	D	359	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

5 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	502	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	B	501	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	D	501	-	4,4,4	0.16	0	6,6,6	0.06	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.

No monomer is involved in short contacts.

## 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	379/404 (93%)	0.74	21 (5%) 25 30	37, 51, 71, 86	0
1	B	380/404 (94%)	0.76	26 (6%) 17 21	39, 50, 70, 93	0
1	C	380/404 (94%)	0.76	22 (5%) 23 28	37, 51, 72, 105	0
1	D	381/404 (94%)	0.68	17 (4%) 33 38	39, 51, 72, 116	0
All	All	1520/1616 (94%)	0.73	86 (5%) 23 28	37, 51, 72, 116	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	23	SER	12.0
1	D	22	ALA	5.8
1	B	23	SER	5.5
1	B	378	VAL	5.1
1	D	23	SER	4.4
1	D	46	LYS	3.9
1	A	50	ARG	3.8
1	D	42	GLN	3.8
1	B	48	VAL	3.7
1	C	344	ASN	3.7
1	B	349	LYS	3.7
1	C	276[A]	MET	3.6
1	B	50	ARG	3.6
1	B	57	LYS	3.6
1	A	210	PRO	3.5
1	B	344	ASN	3.5
1	D	43	LYS	3.2
1	B	362	ALA	3.2
1	C	283	ASP	3.2
1	A	344	ASN	3.1
1	C	50	ARG	3.1

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	342	TYR	3.1
1	A	343	LEU	3.0
1	C	293	THR	2.9
1	D	40	ASP	2.9
1	B	384	ILE	2.9
1	A	361	ALA	2.9
1	C	154	LEU	2.9
1	D	255	LEU	2.8
1	A	306	LEU	2.8
1	A	330	VAL	2.7
1	C	77	PRO	2.7
1	C	24	ALA	2.7
1	B	373	GLY	2.7
1	D	296	LEU	2.7
1	B	343	LEU	2.7
1	D	48	VAL	2.6
1	C	378	VAL	2.6
1	D	349	LYS	2.6
1	C	176	PRO	2.6
1	B	115	VAL	2.6
1	B	43	LYS	2.5
1	C	175	VAL	2.5
1	C	249	ALA	2.5
1	B	25	PRO	2.5
1	C	179	LYS	2.5
1	B	390	THR	2.5
1	B	286	LEU	2.5
1	C	255	LEU	2.5
1	C	348	TRP	2.5
1	C	384	ILE	2.5
1	C	349	LYS	2.4
1	D	321	TRP	2.4
1	A	396	ILE	2.4
1	A	206	LYS	2.4
1	B	312	ILE	2.3
1	B	294	LEU	2.3
1	A	389	SER	2.3
1	D	37	LEU	2.3
1	A	135	GLY	2.3
1	D	258	LEU	2.3
1	A	383	ARG	2.3
1	C	343	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	353	ILE	2.3
1	D	399	LEU	2.2
1	C	346	GLU	2.2
1	A	221	THR	2.2
1	C	288	GLN	2.2
1	B	46	LYS	2.2
1	A	254	VAL	2.2
1	B	350	PHE	2.2
1	B	211	SER	2.2
1	A	340	PRO	2.2
1	A	349	LYS	2.1
1	D	50	ARG	2.1
1	B	244	GLY	2.1
1	D	264	ILE	2.1
1	B	192	PHE	2.1
1	B	364	LEU	2.1
1	D	136	VAL	2.1
1	A	40	ASP	2.0
1	B	45	GLU	2.0
1	A	207	SER	2.0
1	A	63	ILE	2.0
1	A	264	ILE	2.0
1	A	364	LEU	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.

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	501	5/5	0.94	0.13	57,58,61,66	0
2	SO4	B	502	5/5	0.95	0.10	49,52,57,60	0
2	SO4	A	501	5/5	0.95	0.13	54,61,64,68	0
2	SO4	D	501	5/5	0.97	0.12	57,62,64,64	0
2	SO4	B	501	5/5	0.99	0.14	54,58,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.