



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 01:09 am BST

PDB ID : 1W18  
Title : Crystal Structure of levansucrase from *Gluconacetobacter diazotrophicus*  
Authors : Martinez-Fleites, C.; Ortiz-Lombardia, M.; Pons, T.; Tarbouriech, N.; Taylor, E.J.; Hernandez, L.; Davies, G.J.  
Deposited on : 2004-06-16  
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

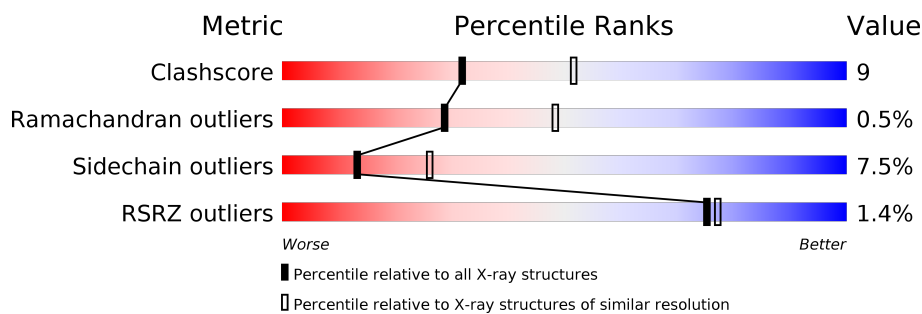
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	493	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>.</div> </div> </div>
1	B	493	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7848 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 LEVANSUCRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3815	2409	668	729	9			
1	B	493	Total	C	N	O	S	0	0	0
			3820	2412	669	730	9			

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



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

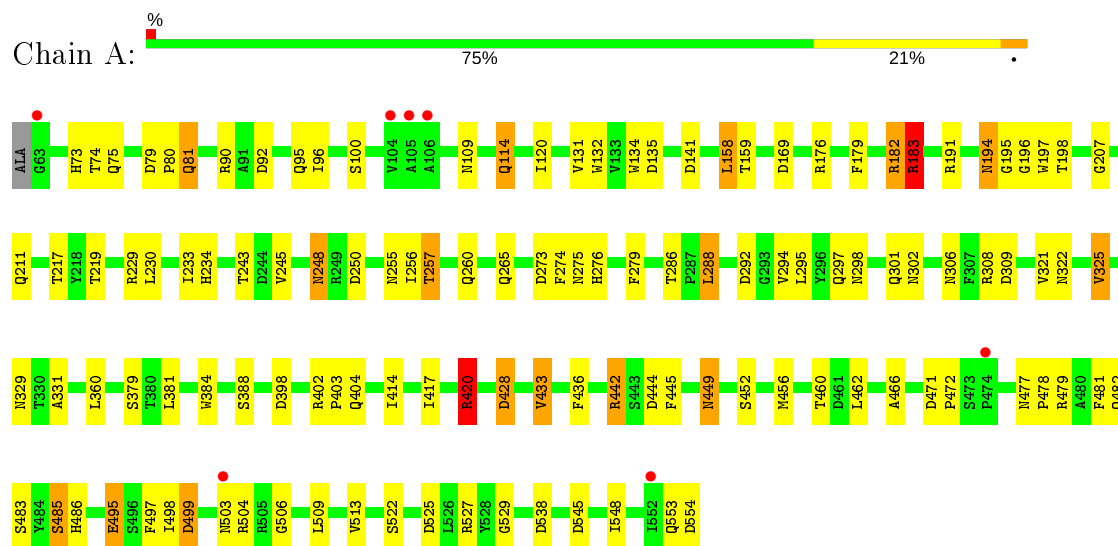
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total 112	O 112	0	0
3	B	81	Total 81	O 81	0	0

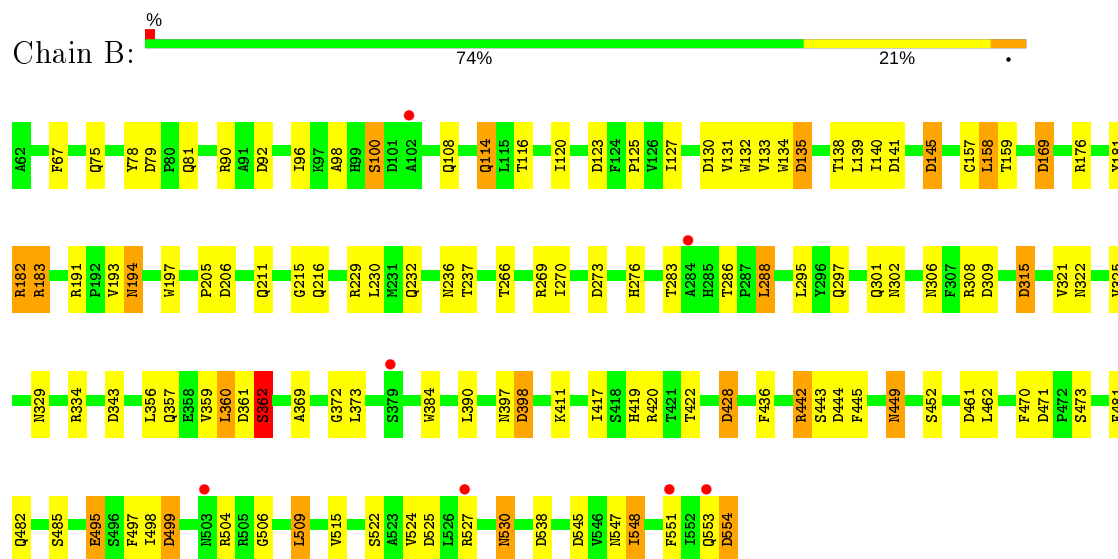
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: LEVANSUCRASE



#### • Molecule 1: LEVANSUCRASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.80Å 119.39Å 215.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.41 – 2.50 52.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (105.41-2.50) 99.0 (52.19-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.14 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0001	Depositor
R, $R_{free}$	0.197 , 0.250 0.210 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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

### 5.1 Standard geometry

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	0.75	2/3930 (0.1%)	0.93	20/5373 (0.4%)
1	B	0.61	0/3935	0.89	25/5380 (0.5%)
All	All	0.68	2/7865 (0.0%)	0.91	45/10753 (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	3
1	B	0	3
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	ALA	CA-CB	6.12	1.65	1.52
1	A	274	PHE	C-O	5.30	1.33	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ASP	CB-CG-OD2	8.24	125.72	118.30
1	A	250	ASP	CB-CG-OD2	8.09	125.58	118.30
1	A	183	ARG	NE-CZ-NH1	-7.82	116.39	120.30
1	B	273	ASP	CB-CG-OD2	7.56	125.10	118.30
1	B	442	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	B	123	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	79	ASP	CB-CG-OD2	6.78	124.40	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	499	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	471	ASP	CB-CG-OD2	6.65	124.28	118.30
1	B	343	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	292	ASP	CB-CG-OD2	6.59	124.23	118.30
1	B	315	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	92	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	141	ASP	CB-CG-OD2	6.43	124.09	118.30
1	A	183	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	B	545	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	442	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	A	545	ASP	CB-CG-OD2	6.16	123.85	118.30
1	B	206	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	398	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	90	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	B	428	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	471	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	428	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	444	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	169	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	444	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	442	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	B	141	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	554	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	538	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	273	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	145	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	176	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	130	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	169	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	79	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	90	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	538	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	461	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	420	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	B	361	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	309	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	499	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	398	ASP	CB-CG-OD2	5.02	122.81	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	207	GLY	Peptide
1	A	275	ASN	Peptide
1	A	553	GLN	Peptide
1	B	205	PRO	Peptide
1	B	215	GLY	Peptide
1	B	553	GLN	Peptide

## 5.2 Too-close contacts ⓘ

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	3815	0	3552	65	0
1	B	3820	0	3557	67	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	112	0	0	5	0
3	B	81	0	0	3	0
All	All	7848	0	7109	132	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 9.

All (132) 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:449:ASN:HD21	1:A:522:SER:H	1.28	0.82
1:A:229:ARG:HH22	1:A:322:ASN:HD21	1.29	0.80
1:A:306:ASN:H	1:A:329:ASN:ND2	1.82	0.78
1:B:449:ASN:HD21	1:B:522:SER:H	1.31	0.78
1:A:135:ASP:HB2	1:A:158:LEU:HD22	1.70	0.74
1:B:525:ASP:OD1	1:B:527:ARG:HG2	1.87	0.74
1:A:229:ARG:HH22	1:A:322:ASN:ND2	1.85	0.73
1:A:309:ASP:OD1	3:A:2063:HOH:O	2.06	0.72
1:A:306:ASN:HD22	1:A:308:ARG:HH12	1.38	0.71
1:A:388:SER:O	1:A:442:ARG:NH1	2.25	0.70
1:B:306:ASN:H	1:B:329:ASN:HD22	1.36	0.70
1:A:306:ASN:H	1:A:329:ASN:HD22	1.43	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:PHE:O	1:B:554:ASP:N	2.29	0.66
1:A:229:ARG:HD2	3:A:2065:HOH:O	1.94	0.66
1:A:120:ILE:H	1:A:482:GLN:HE22	1.42	0.66
1:B:306:ASN:H	1:B:329:ASN:ND2	1.93	0.65
1:B:397:ASN:OD1	1:B:422:THR:HG23	1.96	0.65
1:B:359:VAL:O	1:B:362:SER:HB2	1.97	0.64
1:A:325:VAL:HG13	1:A:403:PRO:HB2	1.79	0.63
1:B:498:ILE:O	1:B:506:GLY:O	2.17	0.63
1:B:229:ARG:HH22	1:B:322:ASN:ND2	1.97	0.63
1:B:127:ILE:HD12	1:B:509:LEU:HD22	1.81	0.61
1:A:498:ILE:O	1:A:506:GLY:O	2.19	0.60
1:A:194:ASN:C	1:A:194:ASN:HD22	2.04	0.60
1:A:420:ARG:HD2	1:A:428:ASP:OD2	2.01	0.60
1:B:306:ASN:HD22	1:B:308:ARG:HH12	1.49	0.60
1:B:417:ILE:CD1	1:B:485:SER:HA	2.32	0.60
1:B:357:GLN:HB3	3:B:2056:HOH:O	2.01	0.59
1:A:306:ASN:HD22	1:A:308:ARG:NH1	2.01	0.59
1:A:194:ASN:C	1:A:194:ASN:ND2	2.55	0.58
1:B:116:THR:O	1:B:524:VAL:HG21	2.04	0.57
1:A:120:ILE:H	1:A:482:GLN:NE2	2.02	0.57
1:B:229:ARG:HH22	1:B:322:ASN:HD21	1.52	0.57
1:A:81:GLN:HA	1:A:81:GLN:HE21	1.69	0.57
1:B:419:HIS:O	1:B:422:THR:HG22	2.05	0.57
1:A:483:SER:OG	1:A:486:HIS:NE2	2.37	0.56
1:B:194:ASN:OD1	3:B:2019:HOH:O	2.18	0.56
1:A:194:ASN:ND2	1:A:196:GLY:H	2.04	0.56
1:B:315:ASP:OD1	3:B:2044:HOH:O	2.18	0.55
1:A:80:PRO:O	1:A:442:ARG:NH2	2.40	0.55
1:A:477:ASN:OD1	1:A:478:PRO:HD2	2.06	0.55
1:A:298:ASN:OD1	1:A:301:GLN:HG3	2.07	0.55
1:B:134:TRP:HB2	1:B:497:PHE:CE1	2.41	0.55
1:B:302:ASN:OD1	1:B:334:ARG:HD2	2.07	0.54
1:B:169:ASP:OD2	1:B:470:PHE:HB3	2.08	0.54
1:A:481:PHE:O	1:A:499:ASP:HB3	2.08	0.54
1:B:306:ASN:HD22	1:B:308:ARG:NH1	2.05	0.54
1:A:183:ARG:O	1:A:191:ARG:NH2	2.41	0.54
1:A:288:LEU:HG	1:A:384:TRP:CD1	2.42	0.53
1:B:288:LEU:HG	1:B:384:TRP:CD1	2.43	0.53
1:A:109:ASN:HD22	1:A:460:THR:H	1.56	0.53
1:A:114:GLN:H	1:A:114:GLN:NE2	2.07	0.52
1:B:183:ARG:O	1:B:191:ARG:NH2	2.42	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLN:NE2	1:B:237:THR:OG1	2.43	0.52
1:B:436:PHE:HB3	1:B:445:PHE:HB3	1.91	0.52
1:B:135:ASP:HB2	1:B:158:LEU:HD22	1.92	0.51
1:B:417:ILE:HD12	1:B:485:SER:HA	1.93	0.51
1:A:414:ILE:HD13	1:A:445:PHE:CE2	2.46	0.51
1:A:472:PRO:HG2	1:A:503:ASN:HD21	1.76	0.51
1:A:420:ARG:HH11	1:A:466:ALA:HA	1.77	0.50
1:B:297:GLN:HA	1:B:301:GLN:NE2	2.26	0.50
1:A:257:THR:HG23	3:A:2042:HOH:O	2.11	0.50
1:B:297:GLN:NE2	1:B:302:ASN:HD22	2.09	0.50
1:A:436:PHE:HB3	1:A:445:PHE:HB3	1.92	0.50
1:B:297:GLN:HE22	1:B:302:ASN:HD22	1.59	0.50
1:A:134:TRP:HB2	1:A:497:PHE:CD1	2.46	0.50
1:B:420:ARG:HD2	1:B:428:ASP:OD2	2.12	0.50
1:A:182:ARG:HD2	1:A:197:TRP:CZ3	2.47	0.50
1:A:298:ASN:H	1:A:301:GLN:HE21	1.59	0.49
1:A:255:ASN:HB3	1:A:257:THR:O	2.12	0.49
1:A:219:THR:HG23	1:A:248:ASN:HD22	1.77	0.48
1:A:402:ARG:N	1:A:403:PRO:CD	2.75	0.48
1:B:369:ALA:HB2	1:B:398:ASP:C	2.33	0.48
1:A:95:GLN:OE1	3:A:2011:HOH:O	2.20	0.48
1:A:243:THR:HG21	1:A:308:ARG:HB3	1.96	0.47
1:A:265:GLN:HB2	1:A:288:LEU:HD21	1.97	0.47
1:B:373:LEU:HD22	1:B:390:LEU:HD21	1.97	0.47
1:A:297:GLN:HE22	1:A:302:ASN:HD22	1.62	0.47
1:B:132:TRP:O	1:B:159:THR:HA	2.15	0.47
1:B:495:GLU:C	1:B:495:GLU:OE1	2.53	0.47
1:B:140:ILE:HA	1:B:145:ASP:O	2.14	0.47
1:A:233:ILE:HG22	3:A:2036:HOH:O	2.16	0.46
1:B:530:ASN:C	1:B:530:ASN:HD22	2.19	0.46
1:B:96:ILE:HG13	1:B:452:SER:HB2	1.97	0.46
1:A:417:ILE:HD12	1:A:485:SER:HA	1.98	0.46
1:B:182:ARG:HD2	1:B:197:TRP:CH2	2.51	0.46
1:A:286:THR:O	1:A:288:LEU:HD13	2.16	0.45
1:A:134:TRP:O	1:A:135:ASP:C	2.54	0.45
1:B:481:PHE:O	1:B:499:ASP:HB3	2.17	0.44
1:B:236:ASN:O	1:B:269:ARG:HA	2.18	0.44
1:B:133:VAL:HG13	1:B:157:CYS:SG	2.57	0.44
1:B:75:GLN:HE22	1:B:411:LYS:HZ2	1.66	0.44
1:B:138:THR:HG23	1:B:139:LEU:N	2.33	0.44
1:B:78:TYR:HB2	1:B:442:ARG:HG2	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ASN:CG	1:B:334:ARG:HD2	2.38	0.44
1:B:547:ASN:O	1:B:548:ILE:C	2.55	0.44
1:B:67:PHE:CD2	1:B:98:ALA:HB2	2.53	0.44
1:A:132:TRP:O	1:A:159:THR:HA	2.17	0.43
1:B:134:TRP:O	1:B:135:ASP:C	2.54	0.43
1:B:325:VAL:HA	1:B:372:GLY:O	2.18	0.43
1:A:100:SER:HB2	1:A:462:LEU:HD12	2.00	0.43
1:B:482:GLN:O	1:B:498:ILE:HA	2.18	0.43
1:A:211:GLN:HB2	1:A:211:GLN:HE21	1.65	0.43
1:A:96:ILE:HG13	1:A:452:SER:HB2	2.00	0.43
1:A:74:THR:O	1:A:75:GLN:HB2	2.18	0.43
1:A:73:HIS:NE2	1:A:92:ASP:OD1	2.39	0.43
1:A:486:HIS:HA	1:A:495:GLU:O	2.19	0.43
1:A:479:ARG:HG2	1:A:482:GLN:HE21	1.83	0.42
1:A:194:ASN:HD22	1:A:195:GLY:N	2.16	0.42
1:B:236:ASN:HB2	1:B:270:ILE:O	2.19	0.42
1:B:108:GLN:CA	1:B:108:GLN:HE21	2.31	0.42
1:B:114:GLN:HE21	1:B:114:GLN:H	1.67	0.42
1:B:182:ARG:HD2	1:B:197:TRP:CZ3	2.55	0.42
1:B:75:GLN:HE22	1:B:411:LYS:NZ	2.17	0.42
1:B:356:LEU:HG	1:B:360:LEU:HD22	2.02	0.42
1:B:100:SER:HB2	1:B:462:LEU:HD12	2.02	0.42
1:B:286:THR:O	1:B:288:LEU:HD13	2.19	0.42
1:B:297:GLN:HA	1:B:301:GLN:HE22	1.84	0.42
1:A:92:ASP:O	1:A:95:GLN:HG2	2.20	0.41
1:B:125:PRO:HG3	1:B:193:VAL:HG22	2.02	0.41
1:A:297:GLN:NE2	1:A:302:ASN:HD22	2.19	0.41
1:B:75:GLN:NE2	1:B:411:LYS:NZ	2.69	0.41
1:A:245:VAL:HA	1:A:260:GLN:O	2.21	0.41
1:B:120:ILE:H	1:B:482:GLN:HE22	1.68	0.41
1:A:402:ARG:N	1:A:403:PRO:HD2	2.34	0.41
1:B:181:TYR:OH	1:B:276:HIS:HB2	2.20	0.41
1:A:483:SER:HG	1:A:486:HIS:HE2	1.56	0.41
1:A:433:VAL:HG13	1:A:456:MET:HB3	2.03	0.41
1:A:179:PHE:CD1	1:A:279:PHE:HE1	2.39	0.40
1:A:525:ASP:OD1	1:A:527:ARG:HG2	2.21	0.40
1:B:108:GLN:HA	1:B:108:GLN:NE2	2.36	0.40
1:B:306:ASN:ND2	1:B:308:ARG:HH22	2.19	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	490/493 (99%)	460 (94%)	28 (6%)	2 (0%)	34	54
1	B	491/493 (100%)	463 (94%)	25 (5%)	3 (1%)	25	43
All	All	981/986 (100%)	923 (94%)	53 (5%)	5 (0%)	29	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	548	ILE
1	A	529	GLY
1	B	362	SER
1	A	449	ASN
1	B	449	ASN

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/395 (100%)	363 (92%)	32 (8%)	11	23
1	B	395/395 (100%)	368 (93%)	27 (7%)	16	30
All	All	790/790 (100%)	731 (92%)	59 (8%)	13	26

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	114	GLN
1	A	131	VAL
1	A	158	LEU
1	A	182	ARG
1	A	183	ARG
1	A	194	ASN
1	A	198	THR
1	A	217	THR
1	A	230	LEU
1	A	234	HIS
1	A	248	ASN
1	A	256	ILE
1	A	257	THR
1	A	276	HIS
1	A	288	LEU
1	A	294	VAL
1	A	295	LEU
1	A	321	VAL
1	A	325	VAL
1	A	360	LEU
1	A	379	SER
1	A	381	LEU
1	A	404	GLN
1	A	420	ARG
1	A	433	VAL
1	A	485	SER
1	A	495	GLU
1	A	504	ARG
1	A	509	LEU
1	A	513	VAL
1	A	548	ILE
1	B	81	GLN
1	B	100	SER
1	B	114	GLN
1	B	131	VAL
1	B	158	LEU
1	B	176	ARG
1	B	182	ARG
1	B	183	ARG
1	B	194	ASN
1	B	211	GLN
1	B	216	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	230	LEU
1	B	266	THR
1	B	283	THR
1	B	288	LEU
1	B	295	LEU
1	B	321	VAL
1	B	360	LEU
1	B	362	SER
1	B	443	SER
1	B	473	SER
1	B	495	GLU
1	B	504	ARG
1	B	509	LEU
1	B	515	VAL
1	B	530	ASN
1	B	554	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	81	GLN
1	A	95	GLN
1	A	109	ASN
1	A	114	GLN
1	A	194	ASN
1	A	211	GLN
1	A	220	ASN
1	A	248	ASN
1	A	255	ASN
1	A	265	GLN
1	A	297	GLN
1	A	301	GLN
1	A	306	ASN
1	A	322	ASN
1	A	329	ASN
1	A	333	GLN
1	A	399	GLN
1	A	449	ASN
1	A	482	GLN
1	A	503	ASN
1	A	519	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	547	ASN
1	B	75	GLN
1	B	108	GLN
1	B	109	ASN
1	B	114	GLN
1	B	194	ASN
1	B	211	GLN
1	B	220	ASN
1	B	232	GLN
1	B	297	GLN
1	B	301	GLN
1	B	306	ASN
1	B	322	ASN
1	B	329	ASN
1	B	399	GLN
1	B	419	HIS
1	B	449	ASN
1	B	463	ASN
1	B	482	GLN
1	B	530	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	1556	-	4,4,4	0.18	0	6,6,6	0.47	0
2	SO4	A	1555	-	4,4,4	0.16	0	6,6,6	0.31	0
2	SO4	A	1556	-	4,4,4	0.25	0	6,6,6	0.34	0
2	SO4	B	1555	-	4,4,4	0.29	0	6,6,6	0.72	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	492/493 (99%)	-0.08	7 (1%) 75 77	14, 24, 30, 59	0
1	B	493/493 (100%)	0.06	7 (1%) 75 77	19, 26, 32, 65	0
All	All	985/986 (99%)	-0.01	14 (1%) 75 77	14, 25, 31, 65	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	ASN	3.1
1	A	105	ALA	2.8
1	B	379	SER	2.6
1	A	552	ILE	2.5
1	A	474	PRO	2.4
1	A	106	ALA	2.3
1	B	551	PHE	2.3
1	A	63	GLY	2.3
1	B	553	GLN	2.3
1	B	503	ASN	2.2
1	B	284	ALA	2.2
1	A	104	VAL	2.1
1	B	102	ALA	2.1
1	B	527	ARG	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	1555	5/5	0.92	0.14	64,64,67,70	0
2	SO4	B	1556	5/5	0.95	0.22	83,83,84,84	0
2	SO4	A	1556	5/5	0.96	0.20	75,76,76,77	0
2	SO4	A	1555	5/5	0.96	0.09	65,65,66,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.