



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:18 pm GMT

PDB ID : 3LCG  
Title : The D-sialic acid aldolase mutant V251L  
Authors : Chou, C.-Y.; Wang, A.H.-J.; Ko, T.-P.  
Deposited on : 2010-01-11  
Resolution : 1.78 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

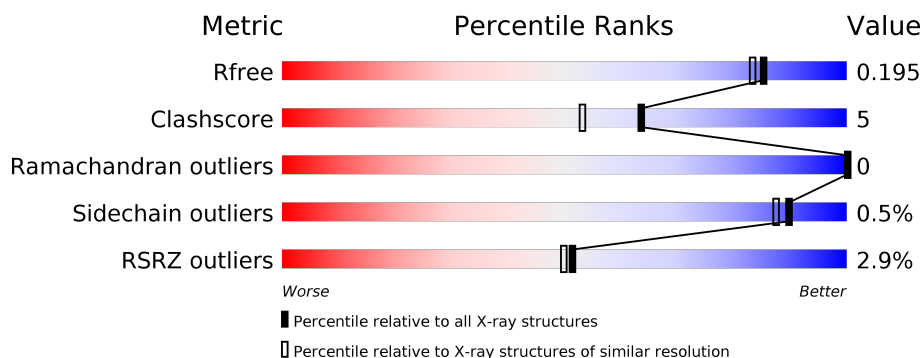
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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))
$R_{free}$	111664	7886 (1.80-1.76)
Clashscore	122126	8858 (1.80-1.76)
Ramachandran outliers	120053	8764 (1.80-1.76)
Sidechain outliers	120020	8763 (1.80-1.76)
RSRZ outliers	108989	7741 (1.80-1.76)

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. 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	319	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>
1	B	319	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>8%</div> </div> </div>
1	C	319	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>8%</div> </div> </div>
1	D	319	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>7%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10806 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 N-acetylneuraminate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2268	1446	384	428	10			
1	B	295	Total	C	N	O	S	0	0	0
			2280	1453	386	431	10			
1	C	294	Total	C	N	O	S	0	0	0
			2275	1450	385	430	10			
1	D	296	Total	C	N	O	S	0	0	0
			2288	1458	387	432	11			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP P0A6L4
A	-20	GLY	-	EXPRESSION TAG	UNP P0A6L4
A	-19	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-18	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-17	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-16	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-15	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-14	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-13	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-12	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-11	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-10	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-9	SER	-	EXPRESSION TAG	UNP P0A6L4
A	-8	SER	-	EXPRESSION TAG	UNP P0A6L4
A	-7	GLY	-	EXPRESSION TAG	UNP P0A6L4
A	-6	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-5	ILE	-	EXPRESSION TAG	UNP P0A6L4
A	-4	GLU	-	EXPRESSION TAG	UNP P0A6L4
A	-3	GLY	-	EXPRESSION TAG	UNP P0A6L4
A	-2	ARG	-	EXPRESSION TAG	UNP P0A6L4
A	-1	HIS	-	EXPRESSION TAG	UNP P0A6L4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP P0A6L4
A	251	LEU	VAL	ENGINEERED MUTATION	UNP P0A6L4
B	-21	MET	-	EXPRESSION TAG	UNP P0A6L4
B	-20	GLY	-	EXPRESSION TAG	UNP P0A6L4
B	-19	HIS	-	EXPRESSION TAG	UNP P0A6L4
B	-18	HIS	-	EXPRESSION TAG	UNP P0A6L4
B	-17	HIS	-	EXPRESSION TAG	UNP P0A6L4
B	-16	HIS	-	EXPRESSION TAG	UNP P0A6L4
B	-15	HIS	-	EXPRESSION TAG	UNP P0A6L4
B	-14	HIS	-	EXPRESSION TAG	UNP P0A6L4
B	-13	HIS	-	EXPRESSION TAG	UNP P0A6L4
B	-12	HIS	-	EXPRESSION TAG	UNP P0A6L4
B	-11	HIS	-	EXPRESSION TAG	UNP P0A6L4
B	-10	HIS	-	EXPRESSION TAG	UNP P0A6L4
B	-9	SER	-	EXPRESSION TAG	UNP P0A6L4
B	-8	SER	-	EXPRESSION TAG	UNP P0A6L4
B	-7	GLY	-	EXPRESSION TAG	UNP P0A6L4
B	-6	HIS	-	EXPRESSION TAG	UNP P0A6L4
B	-5	ILE	-	EXPRESSION TAG	UNP P0A6L4
B	-4	GLU	-	EXPRESSION TAG	UNP P0A6L4
B	-3	GLY	-	EXPRESSION TAG	UNP P0A6L4
B	-2	ARG	-	EXPRESSION TAG	UNP P0A6L4
B	-1	HIS	-	EXPRESSION TAG	UNP P0A6L4
B	0	MET	-	EXPRESSION TAG	UNP P0A6L4
B	251	LEU	VAL	ENGINEERED MUTATION	UNP P0A6L4
C	-21	MET	-	EXPRESSION TAG	UNP P0A6L4
C	-20	GLY	-	EXPRESSION TAG	UNP P0A6L4
C	-19	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-18	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-17	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-16	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-15	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-14	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-13	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-12	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-11	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-10	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-9	SER	-	EXPRESSION TAG	UNP P0A6L4
C	-8	SER	-	EXPRESSION TAG	UNP P0A6L4
C	-7	GLY	-	EXPRESSION TAG	UNP P0A6L4
C	-6	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-5	ILE	-	EXPRESSION TAG	UNP P0A6L4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLU	-	EXPRESSION TAG	UNP P0A6L4
C	-3	GLY	-	EXPRESSION TAG	UNP P0A6L4
C	-2	ARG	-	EXPRESSION TAG	UNP P0A6L4
C	-1	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	0	MET	-	EXPRESSION TAG	UNP P0A6L4
C	251	LEU	VAL	ENGINEERED MUTATION	UNP P0A6L4
D	-21	MET	-	EXPRESSION TAG	UNP P0A6L4
D	-20	GLY	-	EXPRESSION TAG	UNP P0A6L4
D	-19	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	-18	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	-17	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	-16	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	-15	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	-14	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	-13	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	-12	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	-11	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	-10	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	-9	SER	-	EXPRESSION TAG	UNP P0A6L4
D	-8	SER	-	EXPRESSION TAG	UNP P0A6L4
D	-7	GLY	-	EXPRESSION TAG	UNP P0A6L4
D	-6	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	-5	ILE	-	EXPRESSION TAG	UNP P0A6L4
D	-4	GLU	-	EXPRESSION TAG	UNP P0A6L4
D	-3	GLY	-	EXPRESSION TAG	UNP P0A6L4
D	-2	ARG	-	EXPRESSION TAG	UNP P0A6L4
D	-1	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	0	MET	-	EXPRESSION TAG	UNP P0A6L4
D	251	LEU	VAL	ENGINEERED MUTATION	UNP P0A6L4

- 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	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	C	1	Total	O	S	0	0
			5	4	1		
2	D	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	424	Total	O	0	0
			424	424		
3	B	448	Total	O	0	0
			448	448		
3	C	377	Total	O	0	0
			377	377		
3	D	406	Total	O	0	0
			406	406		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.26Å 121.26Å 197.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.01 – 1.78 28.01 – 1.78	Depositor EDS
% Data completeness (in resolution range)	92.0 (28.01-1.78) 96.9 (28.01-1.78)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.99 (at 1.78Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.173 , 0.195 0.173 , 0.195	Depositor DCC
$R_{free}$ test set	7862 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10806	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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	0.30	0/2308	0.60	1/3123 (0.0%)
1	B	0.29	0/2320	0.58	0/3140
1	C	0.29	0/2315	0.57	0/3133
1	D	0.30	0/2328	0.59	1/3150 (0.0%)
All	All	0.29	0/9271	0.59	2/12546 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	GLY	N-CA-C	-5.31	99.82	113.10
1	D	250	GLY	N-CA-C	-5.15	100.22	113.10

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	2268	0	2290	18	0
1	B	2280	0	2302	26	0
1	C	2275	0	2297	26	0
1	D	2288	0	2314	25	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	424	0	0	2	0
3	B	448	0	0	4	0
3	C	377	0	0	2	0
3	D	406	0	0	2	0
All	All	10806	0	9203	84	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 5.

All (84) 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:171:LEU:HD12	1:D:171:LEU:HD12	1.72	0.72
1:A:171:LEU:HD12	1:C:171:LEU:HD12	1.73	0.71
1:B:284:GLU:HG3	3:B:1404:HOH:O	1.93	0.69
1:B:224:LEU:O	1:D:229:ILE:HD12	1.95	0.67
1:A:229:ILE:HD12	1:C:224:LEU:O	1.95	0.67
1:A:64:GLU:O	1:A:68:GLU:HG3	1.96	0.65
1:A:218:GLN:HE21	1:A:218:GLN:HA	1.63	0.64
1:D:51:ALA:HA	1:D:54:GLN:HE21	1.65	0.62
1:A:230:GLN:O	1:A:234:LYS:HG2	1.99	0.61
1:A:290:GLN:O	1:A:294:GLN:HG2	2.01	0.59
1:D:64:GLU:O	1:D:68:GLU:HG3	2.02	0.59
1:B:51:ALA:HA	1:B:54:GLN:HE21	1.65	0.59
1:B:290:GLN:O	1:B:294:GLN:HG2	2.06	0.56
1:D:37:GLN:HB3	1:D:296:ARG:CZ	2.36	0.55
1:C:137:TYR:CE1	1:C:165:LYS:HD3	2.42	0.55
1:B:286:LYS:O	1:B:290:GLN:HG2	2.06	0.55
1:A:137:TYR:CE1	1:A:165:LYS:HD3	2.41	0.55
1:C:286:LYS:O	1:C:290:GLN:HG2	2.07	0.54
1:B:9:MET:O	1:B:206:ILE:HA	2.08	0.54
1:D:106:VAL:HA	1:D:137:TYR:HB3	1.91	0.52
1:A:112:PRO:HG3	3:A:1612:HOH:O	2.09	0.52
1:A:106:VAL:HA	1:A:137:TYR:HB3	1.91	0.51
1:C:139:ILE:HG23	1:C:139:ILE:O	2.10	0.51
1:D:137:TYR:CE1	1:D:165:LYS:HD3	2.46	0.51
1:A:146:LYS:HG3	1:A:146:LYS:O	2.11	0.51
1:C:106:VAL:HA	1:C:137:TYR:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:THR:O	1:D:3:THR:HG22	2.11	0.50
1:B:55:SER:OG	1:B:58:GLU:HG3	2.12	0.50
1:D:9:MET:O	1:D:206:ILE:HA	2.12	0.49
1:B:273:PRO:HG2	1:C:113:PHE:CE1	2.48	0.49
1:B:106:VAL:HA	1:B:137:TYR:HB3	1.94	0.48
1:B:112:PRO:HG3	3:B:1229:HOH:O	2.12	0.48
1:C:56:LEU:O	1:C:60:GLU:HG3	2.12	0.48
1:B:146:LYS:HE3	3:B:1737:HOH:O	2.14	0.48
1:B:90:GLN:NE2	3:B:1177:HOH:O	2.47	0.48
1:B:137:TYR:CE1	1:B:165:LYS:HD3	2.49	0.47
1:A:296:ARG:HD2	3:A:1671:HOH:O	2.13	0.47
1:C:258:VAL:O	1:C:262:MET:HG3	2.14	0.47
1:D:36:GLN:NE2	1:D:36:GLN:HA	2.30	0.47
1:D:19:GLN:O	1:D:20:GLN:HB2	2.15	0.47
1:C:114:SER:OG	1:C:117:GLU:HG3	2.14	0.47
1:D:215:TRP:CZ3	1:D:296:ARG:HD2	2.50	0.47
1:A:156:VAL:HA	1:A:161:VAL:HG11	1.97	0.46
1:B:113:PHE:CZ	1:C:273:PRO:HG2	2.51	0.46
1:A:229:ILE:HG12	1:C:229:ILE:HD11	1.97	0.46
1:C:222:LYS:O	1:C:226:GLU:HG3	2.16	0.46
1:C:9:MET:O	1:C:206:ILE:HA	2.14	0.46
1:D:127:ASP:HB2	3:D:1641:HOH:O	2.15	0.46
1:C:248:LYS:HE3	1:C:281:TYR:CE1	2.51	0.45
1:C:115:PHE:CE1	1:C:151:GLN:HB3	2.52	0.45
1:C:290:GLN:HG3	3:C:1908:HOH:O	2.15	0.45
1:A:9:MET:O	1:A:206:ILE:HA	2.16	0.45
1:A:148:THR:OG1	1:A:151:GLN:HG3	2.17	0.45
1:C:80:VAL:HB	1:C:91:LEU:HB2	1.97	0.45
1:B:229:ILE:HD11	1:D:229:ILE:HG12	1.99	0.45
1:B:113:PHE:CE1	1:C:273:PRO:HG2	2.52	0.45
1:D:163:ALA:HB2	1:D:185:VAL:HB	1.99	0.45
1:D:37:GLN:HB3	1:D:296:ARG:NH1	2.32	0.45
1:C:55:SER:OG	1:C:58:GLU:HG3	2.17	0.44
1:B:253:ARG:HG3	1:B:277:VAL:HG22	1.99	0.44
1:A:80:VAL:HB	1:A:91:LEU:HB2	1.98	0.44
1:D:112:PRO:HG3	3:D:895:HOH:O	2.18	0.43
1:D:96:LYS:HD2	1:D:130:ASP:HB3	1.99	0.43
1:B:273:PRO:HG2	1:C:113:PHE:CZ	2.52	0.43
1:B:139:ILE:HG23	1:B:139:ILE:O	2.19	0.43
1:D:245:LEU:O	1:D:249:THR:HG23	2.18	0.43
1:C:282:LEU:HB2	1:C:283:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:ILE:O	1:D:139:ILE:HG23	2.19	0.43
1:B:114:SER:OG	1:B:117:GLU:HG3	2.19	0.43
1:A:20:GLN:NE2	1:A:271:ARG:HA	2.34	0.42
1:C:19:GLN:HA	1:C:19:GLN:NE2	2.35	0.42
1:C:112:PRO:HG3	3:C:1735:HOH:O	2.19	0.42
1:B:156:VAL:HA	1:B:161:VAL:HG11	2.02	0.42
1:B:115:PHE:CE1	1:B:151:GLN:HB3	2.54	0.42
1:B:192:GLU:HG3	1:D:172:TYR:CG	2.55	0.42
1:D:115:PHE:CE1	1:D:151:GLN:HB3	2.55	0.41
1:D:258:VAL:O	1:D:262:MET:HG3	2.20	0.41
1:D:4:ASN:O	1:D:75:LYS:HE2	2.20	0.41
1:A:139:ILE:O	1:A:139:ILE:HG23	2.19	0.41
1:C:278:ASP:OD1	1:C:280:LYS:HG2	2.21	0.41
1:B:258:VAL:O	1:B:262:MET:HG3	2.21	0.41
1:B:80:VAL:HB	1:B:91:LEU:HB2	2.03	0.40
1:C:156:VAL:HA	1:C:161:VAL:HG11	2.02	0.40
1:D:234:LYS:HD3	1:D:234:LYS:O	2.21	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	291/319 (91%)	286 (98%)	5 (2%)	0	100	100
1	B	293/319 (92%)	286 (98%)	7 (2%)	0	100	100
1	C	292/319 (92%)	286 (98%)	6 (2%)	0	100	100
1	D	294/319 (92%)	287 (98%)	7 (2%)	0	100	100
All	All	1170/1276 (92%)	1145 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	242/263 (92%)	240 (99%)	2 (1%)	83	78
1	B	243/263 (92%)	242 (100%)	1 (0%)	92	89
1	C	243/263 (92%)	242 (100%)	1 (0%)	92	89
1	D	244/263 (93%)	243 (100%)	1 (0%)	92	89
All	All	972/1052 (92%)	967 (100%)	5 (0%)	90	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	218	GLN
1	B	166	GLN
1	C	166	GLN
1	D	294	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	20	GLN
1	A	138	ASN
1	A	166	GLN
1	A	173	GLN
1	A	218	GLN
1	B	18	GLN
1	B	54	GLN
1	B	138	ASN
1	B	166	GLN
1	B	173	GLN
1	C	18	GLN
1	C	19	GLN
1	C	138	ASN

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Mol	Chain	Res	Type
1	C	166	GLN
1	C	173	GLN
1	C	291	GLN
1	D	36	GLN
1	D	54	GLN
1	D	290	GLN
1	D	291	GLN
1	D	294	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](#)

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](#)

8 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	A	1912	-	4,4,4	0.35	0	6,6,6	0.10	0
2	SO4	A	2053	-	4,4,4	0.34	0	6,6,6	0.10	0
2	SO4	B	1913	-	4,4,4	0.34	0	6,6,6	0.12	0
2	SO4	B	2048	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	C	1914	-	4,4,4	0.31	0	6,6,6	0.08	0
2	SO4	C	2049	-	4,4,4	0.32	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	D	1915	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	D	2050	-	4,4,4	0.36	0	6,6,6	0.09	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	SO4	A	1912	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2053	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1913	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2048	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1914	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2049	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1915	-	-	0/0/0/0	0/0/0/0
2	SO4	D	2050	-	-	0/0/0/0	0/0/0/0

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	293/319 (91%)	-0.26	6 (2%) 65 65	13, 19, 32, 57	0
1	B	295/319 (92%)	-0.08	10 (3%) 45 44	15, 20, 36, 60	0
1	C	294/319 (92%)	-0.05	9 (3%) 49 47	16, 21, 40, 56	0
1	D	296/319 (92%)	-0.14	9 (3%) 50 48	13, 19, 35, 57	0
All	All	1178/1276 (92%)	-0.13	34 (2%) 51 50	13, 20, 36, 60	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	THR	6.1
1	A	296	ARG	5.7
1	B	2	ALA	5.1
1	B	3	THR	5.1
1	D	296	ARG	4.3
1	C	294	GLN	4.1
1	B	294	GLN	3.7
1	D	1	MET	3.5
1	D	3	THR	3.4
1	D	2	ALA	3.0
1	C	290	GLN	2.9
1	D	72	GLY	2.8
1	B	296	ARG	2.8
1	A	230	GLN	2.8
1	B	227	GLY	2.8
1	B	36	GLN	2.7
1	C	19	GLN	2.7
1	C	279	GLU	2.6
1	C	296	ARG	2.6
1	C	72	GLY	2.5
1	C	18	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	230	GLN	2.4
1	B	279	GLU	2.4
1	A	36	GLN	2.4
1	D	18	GLN	2.2
1	D	294	GLN	2.2
1	D	70	ALA	2.2
1	A	146	LYS	2.2
1	A	4	ASN	2.1
1	B	263	ASP	2.1
1	C	225	LYS	2.1
1	B	97	ARG	2.1
1	A	72	GLY	2.1
1	B	225	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no 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	D	2050	5/5	0.90	0.18	40,41,45,45	0
2	SO4	B	2048	5/5	0.91	0.18	40,42,44,45	0
2	SO4	C	2049	5/5	0.94	0.17	43,43,45,46	0
2	SO4	A	2053	5/5	0.95	0.16	45,45,47,48	0
2	SO4	C	1914	5/5	0.99	0.07	19,20,22,22	0
2	SO4	D	1915	5/5	0.99	0.06	18,18,19,20	0
2	SO4	B	1913	5/5	0.99	0.05	17,19,20,21	0
2	SO4	A	1912	5/5	1.00	0.05	16,17,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.