



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:35 PM GMT

PDB ID : 3ZXD  
Title : wild-type lysenin  
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Deposited on : 2011-08-09  
Resolution : 3.30 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  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

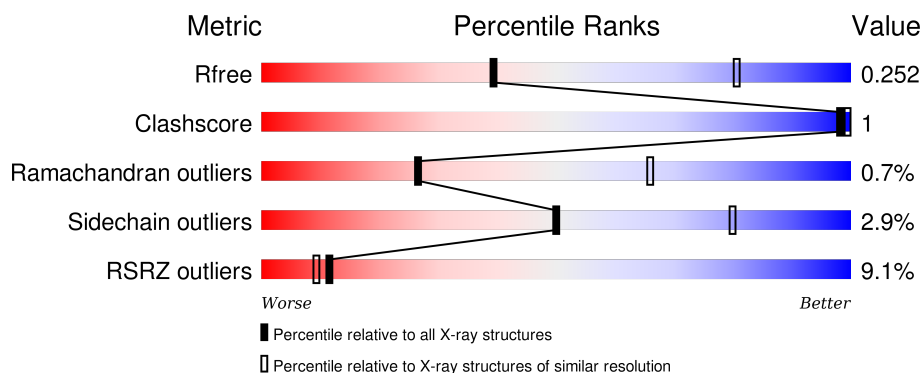
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	309	<div> <div>4%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
1	B	309	<div> <div>5%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
1	C	309	<div> <div>14%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
1	D	309	<div> <div>11%</div> <div>87%</div> <div>6%</div> <div>6%</div> </div>

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	GOL	C	398	-	-	-	X
3	SO4	A	466	-	-	-	X
3	SO4	A	468	-	-	-	X
4	NA	A	467	-	-	-	X
4	NA	D	500	-	-	-	X
7	MES	A	921	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9376 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 LYSENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2330	1476	390	456	8			
1	B	294	Total	C	N	O	S	0	0	0
			2335	1479	391	457	8			
1	C	290	Total	C	N	O	S	0	0	0
			2308	1462	387	451	8			
1	D	289	Total	C	N	O	S	0	0	0
			2304	1460	386	450	8			

There are 52 discrepancies between the modelled and reference sequences:

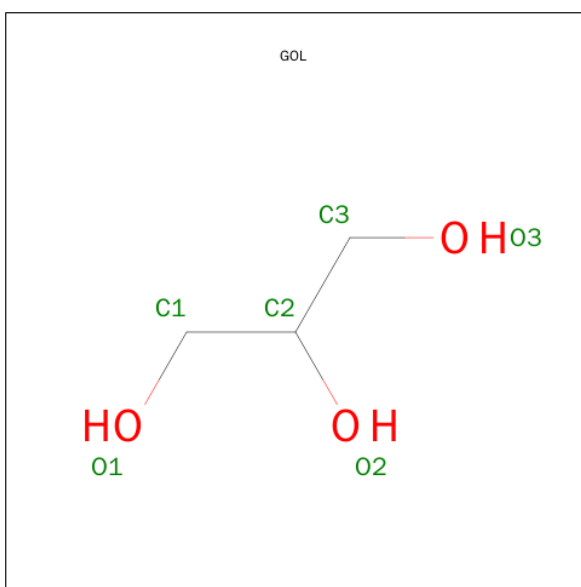
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	LEU	-	EXPRESSION TAG	UNP O18423
A	299	VAL	-	EXPRESSION TAG	UNP O18423
A	300	PRO	-	EXPRESSION TAG	UNP O18423
A	301	ARG	-	EXPRESSION TAG	UNP O18423
A	302	GLY	-	EXPRESSION TAG	UNP O18423
A	303	SER	-	EXPRESSION TAG	UNP O18423
A	304	GLY	-	EXPRESSION TAG	UNP O18423
A	305	HIS	-	EXPRESSION TAG	UNP O18423
A	306	HIS	-	EXPRESSION TAG	UNP O18423
A	307	HIS	-	EXPRESSION TAG	UNP O18423
A	308	HIS	-	EXPRESSION TAG	UNP O18423
A	309	HIS	-	EXPRESSION TAG	UNP O18423
A	310	HIS	-	EXPRESSION TAG	UNP O18423
B	298	LEU	-	EXPRESSION TAG	UNP O18423
B	299	VAL	-	EXPRESSION TAG	UNP O18423
B	300	PRO	-	EXPRESSION TAG	UNP O18423
B	301	ARG	-	EXPRESSION TAG	UNP O18423
B	302	GLY	-	EXPRESSION TAG	UNP O18423
B	303	SER	-	EXPRESSION TAG	UNP O18423
B	304	GLY	-	EXPRESSION TAG	UNP O18423
B	305	HIS	-	EXPRESSION TAG	UNP O18423

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Chain	Residue	Modelled	Actual	Comment	Reference
B	306	HIS	-	EXPRESSION TAG	UNP O18423
B	307	HIS	-	EXPRESSION TAG	UNP O18423
B	308	HIS	-	EXPRESSION TAG	UNP O18423
B	309	HIS	-	EXPRESSION TAG	UNP O18423
B	310	HIS	-	EXPRESSION TAG	UNP O18423
C	298	LEU	-	EXPRESSION TAG	UNP O18423
C	299	VAL	-	EXPRESSION TAG	UNP O18423
C	300	PRO	-	EXPRESSION TAG	UNP O18423
C	301	ARG	-	EXPRESSION TAG	UNP O18423
C	302	GLY	-	EXPRESSION TAG	UNP O18423
C	303	SER	-	EXPRESSION TAG	UNP O18423
C	304	GLY	-	EXPRESSION TAG	UNP O18423
C	305	HIS	-	EXPRESSION TAG	UNP O18423
C	306	HIS	-	EXPRESSION TAG	UNP O18423
C	307	HIS	-	EXPRESSION TAG	UNP O18423
C	308	HIS	-	EXPRESSION TAG	UNP O18423
C	309	HIS	-	EXPRESSION TAG	UNP O18423
C	310	HIS	-	EXPRESSION TAG	UNP O18423
D	298	LEU	-	EXPRESSION TAG	UNP O18423
D	299	VAL	-	EXPRESSION TAG	UNP O18423
D	300	PRO	-	EXPRESSION TAG	UNP O18423
D	301	ARG	-	EXPRESSION TAG	UNP O18423
D	302	GLY	-	EXPRESSION TAG	UNP O18423
D	303	SER	-	EXPRESSION TAG	UNP O18423
D	304	GLY	-	EXPRESSION TAG	UNP O18423
D	305	HIS	-	EXPRESSION TAG	UNP O18423
D	306	HIS	-	EXPRESSION TAG	UNP O18423
D	307	HIS	-	EXPRESSION TAG	UNP O18423
D	308	HIS	-	EXPRESSION TAG	UNP O18423
D	309	HIS	-	EXPRESSION TAG	UNP O18423
D	310	HIS	-	EXPRESSION TAG	UNP O18423

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	4	Total	Na	0	0
			4	4		
4	D	1	Total	Na	0	0
			1	1		

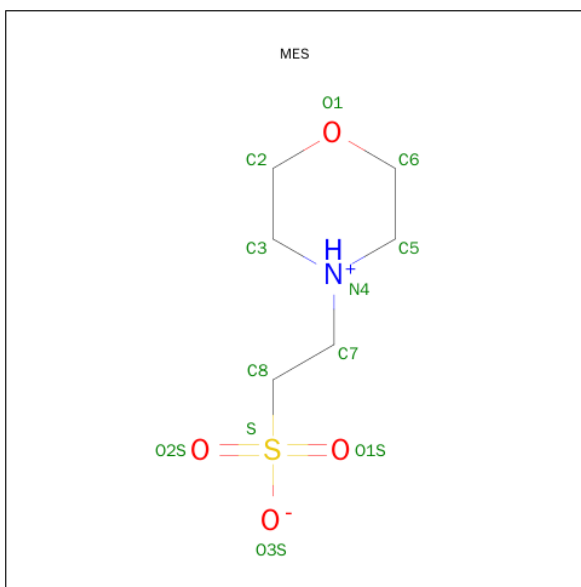
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Mg	0	0
			2	2		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	2	Total	Mg	0	0
			2	2		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is water.

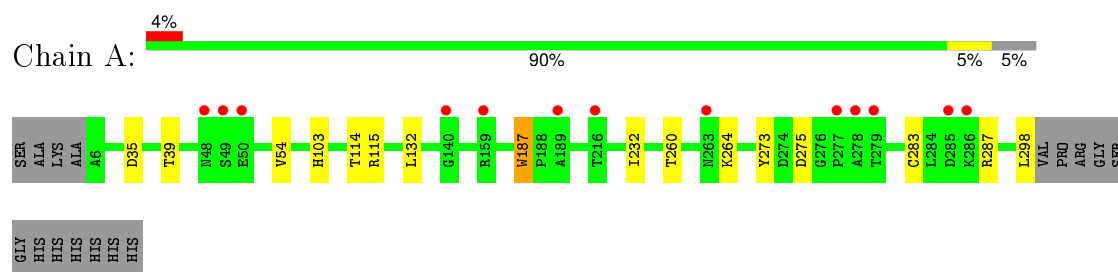
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	O	0	0
			3	3		
8	B	4	Total	O	0	0
			4	4		
8	C	1	Total	O	0	0
			1	1		



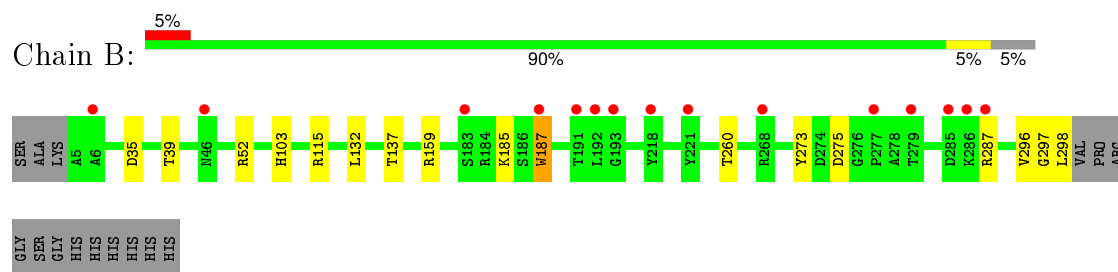
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

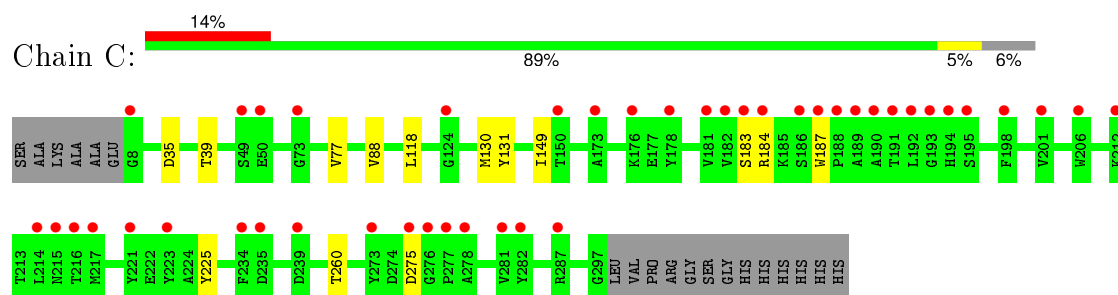
- Molecule 1: LYSENIN



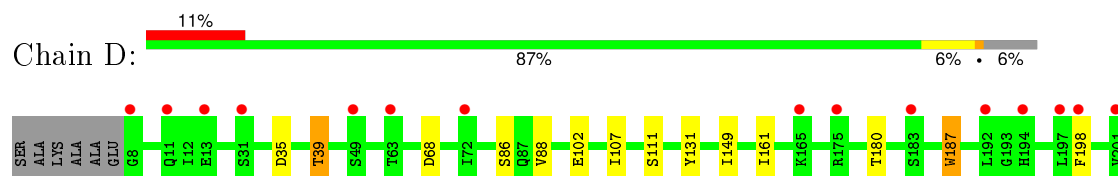
- Molecule 1: LYSENIN

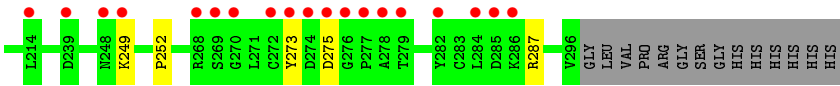


- Molecule 1: LYSENIN



- Molecule 1: LYSENIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.91Å 85.56Å 108.81Å 98.88° 96.84° 90.04°	Depositor
Resolution (Å)	29.09 – 3.30 39.37 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.09-3.30) 92.7 (39.37-3.30)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, $R_{free}$	0.213 , 0.236 0.227 , 0.252	Depositor DCC
$R_{free}$ test set	1542 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.896	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 62.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 30599 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	9376	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CL, NA, SO4, MES

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	0.34	0/2381	0.59	1/3227 (0.0%)
1	B	0.35	0/2386	0.59	1/3234 (0.0%)
1	C	0.35	0/2359	0.56	0/3197
1	D	0.35	0/2355	0.58	1/3192 (0.0%)
All	All	0.35	0/9481	0.58	3/12850 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	187	TRP	CA-CB-CG	5.53	124.21	113.70
1	A	187	TRP	CA-CB-CG	5.50	124.15	113.70
1	B	187	TRP	CA-CB-CG	5.47	124.09	113.70

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	2330	0	2279	4	0
1	B	2335	0	2284	3	0
1	C	2308	0	2257	2	0
1	D	2304	0	2254	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	8	0	0
2	C	6	0	8	0	0
3	A	10	0	0	0	0
3	B	15	0	0	0	0
3	D	5	0	0	0	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
7	A	12	0	13	0	0
7	B	12	0	13	0	0
7	D	12	0	13	3	0
8	A	3	0	0	0	0
8	B	4	0	0	0	0
8	C	1	0	0	0	0
All	All	9376	0	9129	18	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 1.

All (18) 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:C:77:VAL:HG21	1:C:118:LEU:HD21	1.76	0.68
1:D:252:PRO:O	7:D:921:MES:H21	2.00	0.60
1:D:88:VAL:HG11	1:D:131:TYR:CD1	2.48	0.49
1:A:115:ARG:CZ	1:A:132:LEU:HD11	2.43	0.49
1:B:103:HIS:NE2	1:B:115:ARG:NH2	2.57	0.48
1:A:103:HIS:NE2	1:A:115:ARG:NH2	2.58	0.47
1:D:88:VAL:HG11	1:D:131:TYR:CG	2.50	0.47
1:D:273:TYR:O	1:D:287:ARG:NH2	2.50	0.45
1:A:273:TYR:O	1:A:287:ARG:NH2	2.50	0.45
1:B:273:TYR:O	1:B:287:ARG:NH2	2.51	0.44
1:D:107:ILE:HD11	1:D:111:SER:O	2.18	0.43
1:D:68:ASP:HA	7:D:921:MES:H61	1.99	0.43
1:D:249:LYS:HD2	7:D:921:MES:H82	2.02	0.42
1:D:39:THR:HG23	1:D:102:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ILE:HD11	1:A:283:CYS:HB2	2.01	0.41
1:C:88:VAL:HG11	1:C:131:TYR:CD1	2.56	0.41
1:D:180:THR:HA	1:D:198:PHE:HD2	1.86	0.40
1:B:115:ARG:CZ	1:B:132:LEU:HD11	2.51	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	291/309 (94%)	274 (94%)	16 (6%)	1 (0%)	46	81
1	B	292/309 (94%)	276 (94%)	13 (4%)	3 (1%)	19	58
1	C	288/309 (93%)	271 (94%)	14 (5%)	3 (1%)	19	58
1	D	287/309 (93%)	270 (94%)	16 (6%)	1 (0%)	46	81
All	All	1158/1236 (94%)	1091 (94%)	59 (5%)	8 (1%)	26	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	183	SER
1	C	184	ARG
1	B	297	GLY
1	B	185	LYS
1	B	275	ASP
1	D	275	ASP
1	A	275	ASP
1	C	275	ASP

### 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	256/268 (96%)	248 (97%)	8 (3%)	47	79
1	B	256/268 (96%)	247 (96%)	9 (4%)	43	77
1	C	254/268 (95%)	247 (97%)	7 (3%)	51	80
1	D	254/268 (95%)	248 (98%)	6 (2%)	57	83
All	All	1020/1072 (95%)	990 (97%)	30 (3%)	50	80

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	39	THR
1	A	54	VAL
1	A	114	THR
1	A	187	TRP
1	A	260	THR
1	A	264	LYS
1	A	298	LEU
1	B	35	ASP
1	B	39	THR
1	B	52	ARG
1	B	137	THR
1	B	159	ARG
1	B	187	TRP
1	B	260	THR
1	B	296	VAL
1	B	298	LEU
1	C	35	ASP
1	C	39	THR
1	C	130	MET
1	C	149	ILE
1	C	187	TRP
1	C	225	TYR
1	C	260	THR

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Mol	Chain	Res	Type
1	D	35	ASP
1	D	39	THR
1	D	86	SER
1	D	149	ILE
1	D	161	ILE
1	D	187	TRP

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 13 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GOL	A	398	-	5,5,5	0.27	0	5,5,5	0.19	0
3	SO4	A	466	-	4,4,4	3.33	2 (50%)	6,6,6	0.58	0
3	SO4	A	468	6	4,4,4	3.27	2 (50%)	6,6,6	0.58	0
7	MES	A	921	-	11,12,12	0.41	0	14,16,16	1.35	2 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	465	6	4,4,4	3.35	2 (50%)	6,6,6	0.57	0
3	SO4	B	468	-	4,4,4	3.29	2 (50%)	6,6,6	0.57	0
3	SO4	B	473	-	4,4,4	3.39	2 (50%)	6,6,6	0.56	0
7	MES	B	921	-	11,12,12	0.31	0	14,16,16	1.32	2 (14%)
2	GOL	C	398	-	5,5,5	0.47	0	5,5,5	0.29	0
3	SO4	D	467	6	4,4,4	3.39	2 (50%)	6,6,6	0.54	0
7	MES	D	921	-	11,12,12	0.43	0	14,16,16	1.32	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	398	-	-	0/4/4/4	0/0/0/0
3	SO4	A	466	-	-	0/0/0/0	0/0/0/0
3	SO4	A	468	6	-	0/0/0/0	0/0/0/0
7	MES	A	921	-	-	0/6/14/14	0/1/1/1
3	SO4	B	465	6	-	0/0/0/0	0/0/0/0
3	SO4	B	468	-	-	0/0/0/0	0/0/0/0
3	SO4	B	473	-	-	0/0/0/0	0/0/0/0
7	MES	B	921	-	-	0/6/14/14	0/1/1/1
2	GOL	C	398	-	-	0/4/4/4	0/0/0/0
3	SO4	D	467	6	-	0/0/0/0	0/0/0/0
7	MES	D	921	-	-	0/6/14/14	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	468	SO4	O4-S	4.48	1.63	1.47
3	B	468	SO4	O4-S	4.49	1.63	1.47
3	A	466	SO4	O4-S	4.50	1.63	1.47
3	B	465	SO4	O4-S	4.60	1.63	1.47
3	B	473	SO4	O4-S	4.61	1.64	1.47
3	D	467	SO4	O4-S	4.64	1.64	1.47
3	A	468	SO4	O1-S	4.71	1.63	1.47
3	B	468	SO4	O1-S	4.77	1.63	1.47
3	B	465	SO4	O1-S	4.84	1.63	1.47
3	A	466	SO4	O1-S	4.85	1.63	1.47
3	D	467	SO4	O1-S	4.88	1.63	1.47
3	B	473	SO4	O1-S	4.91	1.64	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	921	MES	O2S-S-C8	2.57	109.10	106.91
7	A	921	MES	O2S-S-C8	2.72	109.23	106.91
7	D	921	MES	O2S-S-C8	2.73	109.24	106.91
7	B	921	MES	O1S-S-C8	2.97	109.44	106.91
7	A	921	MES	O1S-S-C8	3.22	109.66	106.91
7	D	921	MES	O1S-S-C8	3.38	109.79	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	921	MES	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	293/309 (94%)	0.28	13 (4%) 38 31	25, 48, 81, 94	0
1	B	294/309 (95%)	0.26	15 (5%) 32 25	22, 50, 98, 121	0
1	C	290/309 (93%)	0.81	44 (15%) 3 2	24, 85, 132, 148	0
1	D	289/309 (93%)	0.66	34 (11%) 6 5	25, 90, 126, 146	0
All	All	1166/1236 (94%)	0.50	106 (9%) 11 9	22, 61, 123, 148	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	182	VAL	5.6
1	C	276	GLY	5.3
1	C	186	SER	5.3
1	C	277	PRO	5.2
1	D	277	PRO	5.2
1	D	273	TYR	5.1
1	C	278	ALA	4.9
1	C	183	SER	4.8
1	C	221	TYR	4.2
1	C	282	TYR	4.2
1	C	181	VAL	4.1
1	D	268	ARG	4.1
1	C	234	PHE	3.9
1	A	286	LYS	3.8
1	D	286	LYS	3.7
1	C	275	ASP	3.7
1	D	285	ASP	3.7
1	C	184	ARG	3.6
1	C	193	GLY	3.6
1	C	176	LYS	3.6
1	C	189	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	11	GLN	3.5
1	C	190	ALA	3.5
1	C	192	LEU	3.5
1	D	269	SER	3.5
1	C	187	TRP	3.5
1	B	191	THR	3.5
1	C	206	TRP	3.4
1	B	279	THR	3.4
1	D	275	ASP	3.4
1	A	278	ALA	3.4
1	B	286	LYS	3.4
1	B	277	PRO	3.3
1	C	217	MET	3.3
1	C	173	ALA	3.2
1	C	235	ASP	3.2
1	B	285	ASP	3.1
1	D	282	TYR	3.1
1	C	216	THR	3.0
1	D	276	GLY	2.9
1	C	223	TYR	2.9
1	C	194	HIS	2.9
1	D	49	SER	2.9
1	C	212	LYS	2.9
1	D	8	GLY	2.9
1	C	195	SER	2.8
1	D	31	SER	2.8
1	D	198	PHE	2.7
1	D	197	LEU	2.7
1	B	6	ALA	2.7
1	C	191	THR	2.7
1	D	248	ASN	2.6
1	C	8	GLY	2.6
1	D	239	ASP	2.6
1	B	192	LEU	2.6
1	C	150	THR	2.6
1	B	183	SER	2.6
1	D	165	LYS	2.5
1	D	175	ARG	2.5
1	C	198	PHE	2.5
1	B	221	TYR	2.5
1	C	49	SER	2.5
1	B	218	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	48	ASN	2.4
1	A	50	GLU	2.4
1	D	194	HIS	2.4
1	C	214	LEU	2.4
1	C	239	ASP	2.4
1	D	279	THR	2.4
1	C	201	VAL	2.4
1	A	189	ALA	2.4
1	D	270	GLY	2.4
1	C	178	TYR	2.4
1	A	277	PRO	2.4
1	C	188	PRO	2.4
1	D	72	ILE	2.4
1	D	278	ALA	2.3
1	C	287	ARG	2.3
1	C	124	GLY	2.3
1	D	272	CYS	2.3
1	D	284	LEU	2.3
1	D	183	SER	2.3
1	C	273	TYR	2.3
1	D	192	LEU	2.3
1	A	279	THR	2.3
1	D	274	ASP	2.3
1	A	159	ARG	2.3
1	C	215	ASN	2.2
1	D	249	LYS	2.2
1	C	73	GLY	2.2
1	A	216	THR	2.2
1	A	263	ASN	2.2
1	A	49	SER	2.2
1	B	287	ARG	2.1
1	B	268	ARG	2.1
1	A	140	GLY	2.1
1	B	193	GLY	2.1
1	C	50	GLU	2.1
1	D	13	GLU	2.1
1	D	63	THR	2.1
1	C	281	VAL	2.1
1	A	285	ASP	2.1
1	B	46	ASN	2.0
1	D	214	LEU	2.0
1	B	187	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	201	VAL	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	C	398	6/6	0.72	0.41	12.09	31,41,44,45	0
4	NA	D	500	1/1	0.80	0.44	10.49	49,49,49,49	0
3	SO4	A	466	5/5	0.82	0.39	3.23	122,122,123,123	0
4	NA	A	467	1/1	0.94	0.22	2.95	25,25,25,25	0
7	MES	A	921	12/12	0.83	0.32	2.16	58,61,67,69	0
3	SO4	A	468	5/5	0.81	0.40	2.12	148,149,151,154	0
3	SO4	D	467	5/5	0.79	0.30	1.36	74,78,80,81	5
3	SO4	B	465	5/5	0.91	0.21	0.21	31,34,36,40	5
7	MES	B	921	12/12	0.90	0.21	-0.05	61,64,71,73	0
7	MES	D	921	12/12	0.64	0.32	-0.06	134,138,144,146	0
4	NA	B	500	1/1	0.94	0.23	-0.24	24,24,24,24	0
2	GOL	A	398	6/6	0.87	0.22	-0.92	55,62,63,67	0
6	MG	C	546	1/1	0.88	0.12	-1.03	44,44,44,44	0
4	NA	A	502	1/1	0.94	0.23	-	40,40,40,40	0
5	CL	A	469	1/1	0.86	0.29	-	61,61,61,61	0
6	MG	D	470	1/1	0.84	0.26	-	32,32,32,32	0
3	SO4	B	468	5/5	0.83	0.33	-	114,116,117,117	0
6	MG	C	547	1/1	0.80	0.24	-	36,36,36,36	0
6	MG	A	470	1/1	0.49	0.74	-	55,55,55,55	0
4	NA	A	500	1/1	0.96	0.53	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	B	472	1/1	0.86	0.20	-	30,30,30,30	0
6	MG	B	470	1/1	0.92	0.16	-	27,27,27,27	0
4	NA	A	501	1/1	0.93	0.14	-	51,51,51,51	0
3	SO4	B	473	5/5	0.84	0.30	-	72,76,76,78	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.