



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:58 AM UTC

PDB ID : 3ZXD / pdb_00003zxd
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

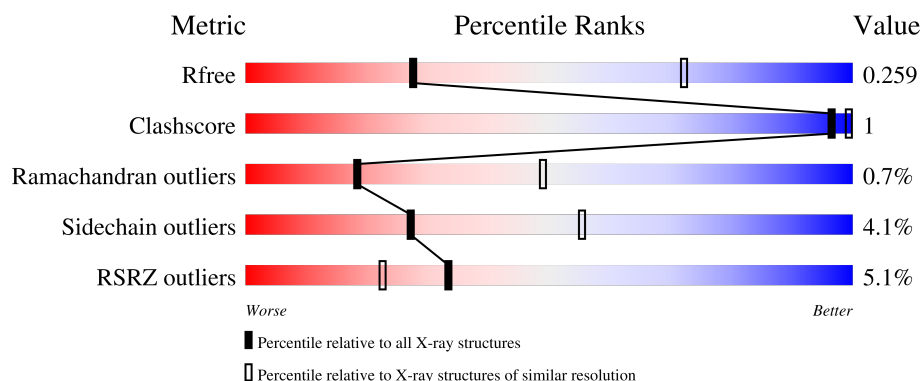
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 ≥ 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	309	2% 89% 6% 5%
1	B	309	4% 88% 7% 5%
1	C	309	8% 88% 6% 6%
1	D	309	5% 86% 6% 6%

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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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 (CCD ID: SO₄) (formula: O₄S).



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 (CCD ID: NA) (formula: Na).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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		

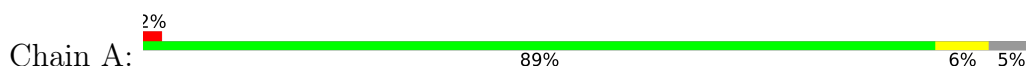
- Molecule 8 is water.

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		

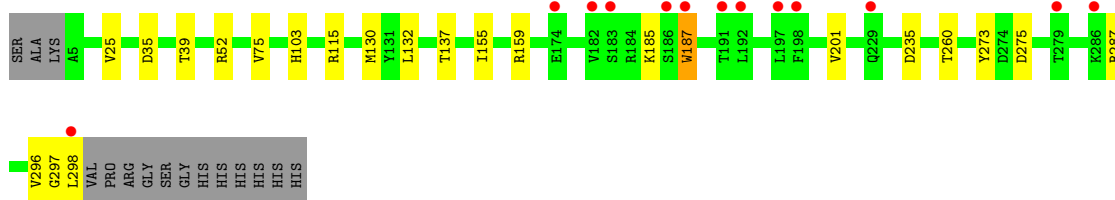
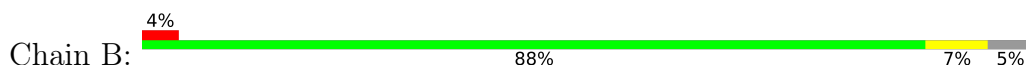
3 Residue-property plots [i](#)

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.

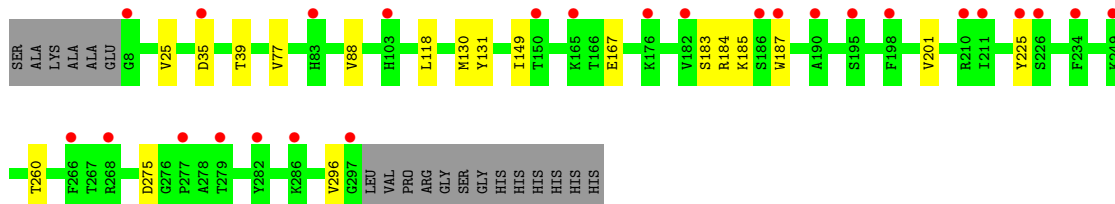
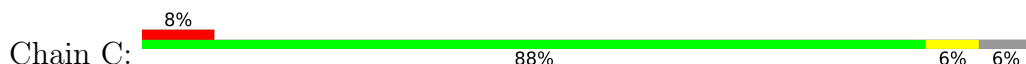
• Molecule 1: LYSENIN



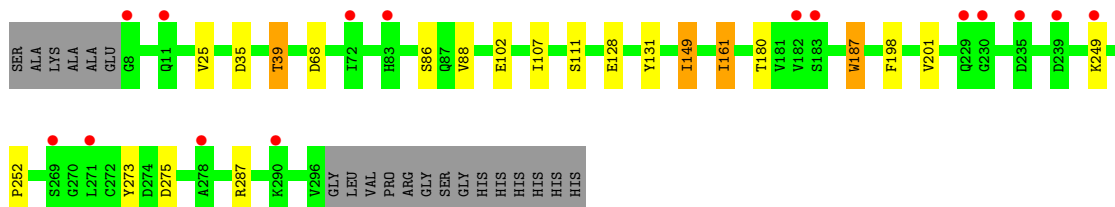
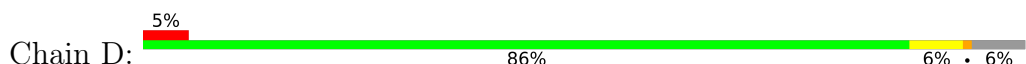
• Molecule 1: LYSENIN



• Molecule 1: LYSENIN



• Molecule 1: LYSENIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.91Å 85.56Å 108.81Å 98.88° 96.84° 90.04°	Depositor
Resolution (Å)	29.09 – 3.30 29.09 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.09-3.30) 97.6 (29.09-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.213 , 0.236 0.236 , 0.259	Depositor DCC
R_{free} test set	1541 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.896	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9376	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, MG, GOL, MES, CL, NA

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	0.68	0/2381	0.98	1/3227 (0.0%)
1	B	0.69	0/2386	0.99	2/3234 (0.1%)
1	C	0.71	1/2359 (0.0%)	0.97	0/3197
1	D	0.68	0/2355	0.98	3/3192 (0.1%)
All	All	0.69	1/9481 (0.0%)	0.98	6/12850 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	185	LYS	CA-C	7.85	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	ILE	N-CA-C	-5.95	106.70	111.81
1	D	187	TRP	CA-CB-CG	5.58	124.21	113.60
1	A	187	TRP	CA-CB-CG	5.55	124.15	113.60
1	B	187	TRP	CA-CB-CG	5.52	124.09	113.60
1	B	235	ASP	CA-CB-CG	5.44	118.04	112.60
1	D	161	ILE	N-CA-CB	5.37	118.13	111.41

There are no chirality outliers.

There are no planarity outliers.

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	2330	0	2279	4	0
1	B	2335	0	2284	4	0
1	C	2308	0	2257	2	0
1	D	2304	0	2254	9	0
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	19	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 (19) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:75:VAL:HG11	1:B:130:MET:HE1	2.04	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%)	36	65
1	B	292/309 (94%)	276 (94%)	13 (4%)	3 (1%)	12	40
1	C	288/309 (93%)	271 (94%)	14 (5%)	3 (1%)	12	40
1	D	287/309 (93%)	270 (94%)	16 (6%)	1 (0%)	36	65
All	All	1158/1236 (94%)	1091 (94%)	59 (5%)	8 (1%)	18	49

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

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Mol	Chain	Res	Type
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%)	246 (96%)	10 (4%)	28	56
1	B	256/268 (96%)	244 (95%)	12 (5%)	23	52
1	C	254/268 (95%)	243 (96%)	11 (4%)	26	54
1	D	254/268 (95%)	245 (96%)	9 (4%)	32	58
All	All	1020/1072 (95%)	978 (96%)	42 (4%)	27	55

All (42) 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	88	VAL
1	A	114	THR
1	A	187	TRP
1	A	201	VAL
1	A	260	THR
1	A	264	LYS
1	A	298	LEU
1	B	25	VAL
1	B	35	ASP
1	B	39	THR
1	B	52	ARG
1	B	137	THR
1	B	155	ILE
1	B	159	ARG
1	B	187	TRP

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Mol	Chain	Res	Type
1	B	201	VAL
1	B	260	THR
1	B	296	VAL
1	B	298	LEU
1	C	25	VAL
1	C	35	ASP
1	C	39	THR
1	C	130	MET
1	C	149	ILE
1	C	167	GLU
1	C	187	TRP
1	C	201	VAL
1	C	225	TYR
1	C	260	THR
1	C	296	VAL
1	D	25	VAL
1	D	35	ASP
1	D	39	THR
1	D	86	SER
1	D	128	GLU
1	D	149	ILE
1	D	161	ILE
1	D	187	TRP
1	D	201	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	GLN
1	B	119	ASN
1	B	194	HIS
1	B	243	GLN
1	C	36	GLN
1	C	119	ASN
1	C	194	HIS
1	C	229	GLN
1	D	87	GLN
1	D	117	GLN
1	D	119	ASN
1	D	194	HIS
1	D	243	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 oligosaccharides 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$
3	SO4	A	466	-	4,4,4	1.86	1 (25%)	6,6,6	0.97	1 (16%)
7	MES	B	921	-	12,12,12	0.81	1 (8%)	15,16,16	1.07	0
2	GOL	C	398	-	5,5,5	0.55	0	5,5,5	0.32	0
7	MES	A	921	-	12,12,12	1.03	1 (8%)	15,16,16	1.07	0
3	SO4	B	468	-	4,4,4	1.83	1 (25%)	6,6,6	0.99	1 (16%)
7	MES	D	921	-	12,12,12	1.02	1 (8%)	15,16,16	1.00	1 (6%)
3	SO4	B	465	6	4,4,4	1.87	1 (25%)	6,6,6	0.96	0
3	SO4	D	467	6	4,4,4	1.88	1 (25%)	6,6,6	0.94	0
2	GOL	A	398	-	5,5,5	0.34	0	5,5,5	0.26	0
3	SO4	B	473	-	4,4,4	1.88	1 (25%)	6,6,6	0.96	0
3	SO4	A	468	6	4,4,4	1.82	1 (25%)	6,6,6	1.00	1 (16%)

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
7	MES	B	921	-	-	2/6/14/14	0/1/1/1
2	GOL	C	398	-	-	0/4/4/4	-
7	MES	A	921	-	-	2/6/14/14	0/1/1/1
7	MES	D	921	-	-	5/6/14/14	0/1/1/1
2	GOL	A	398	-	-	0/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	921	MES	C8-S	3.25	1.82	1.77
3	B	473	SO4	O1-S	3.22	1.64	1.44
3	D	467	SO4	O1-S	3.20	1.63	1.44
3	A	466	SO4	O1-S	3.18	1.63	1.44
3	B	465	SO4	O1-S	3.18	1.63	1.44
7	D	921	MES	C8-S	3.15	1.82	1.77
3	B	468	SO4	O1-S	3.14	1.63	1.44
3	A	468	SO4	O1-S	3.10	1.63	1.44
7	B	921	MES	C8-S	2.53	1.81	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	468	SO4	O3-S-O2	2.07	120.37	109.56
3	B	468	SO4	O3-S-O2	2.04	120.22	109.56
7	D	921	MES	O1S-S-C8	2.03	109.79	106.73
3	A	466	SO4	O3-S-O2	2.01	120.07	109.56

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	921	MES	C8-C7-N4-C3
7	A	921	MES	C8-C7-N4-C5
7	B	921	MES	C8-C7-N4-C3
7	B	921	MES	C8-C7-N4-C5
7	D	921	MES	C8-C7-N4-C5
7	D	921	MES	C7-C8-S-O1S
7	D	921	MES	C7-C8-S-O2S
7	D	921	MES	C7-C8-S-O3S
7	D	921	MES	C8-C7-N4-C3

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, 95th 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 ²)	Q<0.9
1	A	293/309 (94%)	0.39	5 (1%) 69 50	25, 48, 81, 94	0
1	B	294/309 (95%)	0.53	13 (4%) 39 25	22, 50, 98, 121	0
1	C	290/309 (93%)	0.86	26 (8%) 15 11	24, 85, 132, 148	0
1	D	289/309 (93%)	0.74	15 (5%) 33 22	25, 90, 126, 146	0
All	All	1166/1236 (94%)	0.63	59 (5%) 33 22	22, 61, 123, 148	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	ALA	4.0
1	D	8	GLY	3.9
1	B	198	PHE	3.8
1	D	239	ASP	3.8
1	C	198	PHE	3.3
1	B	286	LYS	3.2
1	B	191	THR	3.1
1	C	226	SER	3.0
1	D	229	GLN	3.0
1	C	286	LYS	2.9
1	C	195	SER	2.8
1	B	183	SER	2.8
1	D	72	ILE	2.8
1	C	190	ALA	2.7
1	C	277	PRO	2.6
1	C	8	GLY	2.6
1	C	249	LYS	2.6
1	C	83	HIS	2.6
1	A	298	LEU	2.6
1	C	187	TRP	2.5
1	B	186	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	279	THR	2.5
1	B	182	VAL	2.5
1	C	211	ILE	2.5
1	B	298	LEU	2.5
1	C	182	VAL	2.5
1	D	182	VAL	2.5
1	D	230	GLY	2.4
1	D	11	GLN	2.4
1	B	229	GLN	2.4
1	D	183	SER	2.4
1	D	249	LYS	2.3
1	D	278	ALA	2.3
1	C	297	GLY	2.3
1	C	268	ARG	2.3
1	D	271	LEU	2.3
1	B	279	THR	2.3
1	A	124	GLY	2.3
1	C	165	LYS	2.3
1	C	210	ARG	2.3
1	C	186	SER	2.2
1	C	282	TYR	2.2
1	D	235	ASP	2.2
1	B	197	LEU	2.2
1	A	186	SER	2.2
1	C	103	HIS	2.2
1	B	192	LEU	2.2
1	C	234	PHE	2.1
1	D	83	HIS	2.1
1	C	176	LYS	2.1
1	B	174	GLU	2.1
1	D	269	SER	2.1
1	C	35	ASP	2.1
1	C	225	TYR	2.1
1	C	266	PHE	2.1
1	C	150	THR	2.1
1	C	279	THR	2.1
1	B	187	TRP	2.0
1	D	290	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	A	470	1/1	0.48	0.20	55,55,55,55	0
7	MES	D	921	12/12	0.64	0.26	134,138,144,146	0
6	MG	B	472	1/1	0.71	0.08	30,30,30,30	0
3	SO4	A	468	5/5	0.71	0.28	148,149,151,154	0
3	SO4	B	468	5/5	0.73	0.19	114,116,117,117	0
2	GOL	C	398	6/6	0.75	0.22	31,41,44,45	0
3	SO4	D	467	5/5	0.79	0.17	74,78,80,81	5
3	SO4	A	466	5/5	0.81	0.28	122,122,123,123	0
7	MES	A	921	12/12	0.83	0.19	58,61,67,69	0
7	MES	B	921	12/12	0.89	0.14	61,64,71,73	0
6	MG	C	546	1/1	0.89	0.09	44,44,44,44	0
2	GOL	A	398	6/6	0.90	0.12	55,62,63,67	0
3	SO4	B	473	5/5	0.91	0.14	72,76,76,78	5
4	NA	A	501	1/1	0.91	0.11	51,51,51,51	0
4	NA	D	500	1/1	0.91	0.14	49,49,49,49	0
6	MG	B	470	1/1	0.92	0.05	27,27,27,27	0
5	CL	A	469	1/1	0.92	0.09	61,61,61,61	0
3	SO4	B	465	5/5	0.92	0.12	31,34,36,40	5
4	NA	B	500	1/1	0.93	0.13	24,24,24,24	0
6	MG	D	470	1/1	0.95	0.15	32,32,32,32	0
4	NA	A	500	1/1	0.95	0.16	59,59,59,59	0
4	NA	A	467	1/1	0.96	0.09	25,25,25,25	0
4	NA	A	502	1/1	0.97	0.06	40,40,40,40	0
6	MG	C	547	1/1	0.97	0.05	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.