Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 10:53 pm GMT

PDB ID	:	3ZXD
Title	:	wild-type lysenin
Authors	:	De Colibus, L.; Sonnen, A.F.P.; Morris, K.J.; Siebert, C.A.; Abrusci, P.; Plitzko, J.; Hodnik, V.; Leippe, M.; Volpi, E.; Anderluh, G.; Gilbert, R.J.C.
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 (i) 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 (i)) were used in the production of this report:

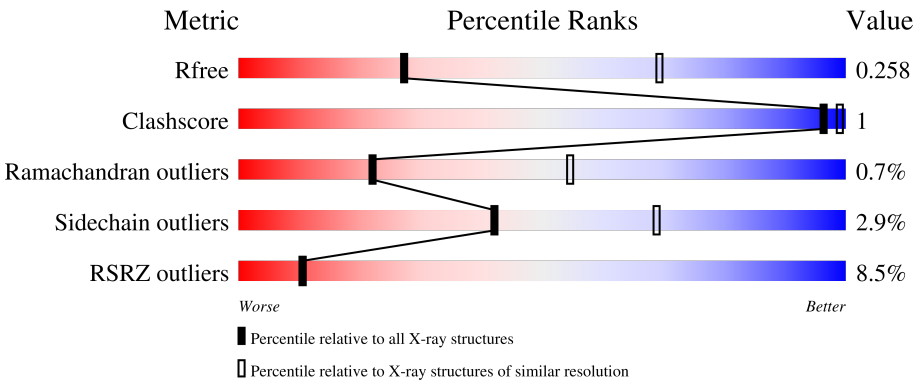
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	4% 90% 5% 5%
1	B	309	4% 90% 5% 5%
1	C	309	14% 89% 5% 6%
1	D	309	10% 87% 6% • 6%

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
6	MG	A	470	-	-	-	X

2 Entry composition (i)

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

There are 52 discrepancies between the modelled and reference sequences:

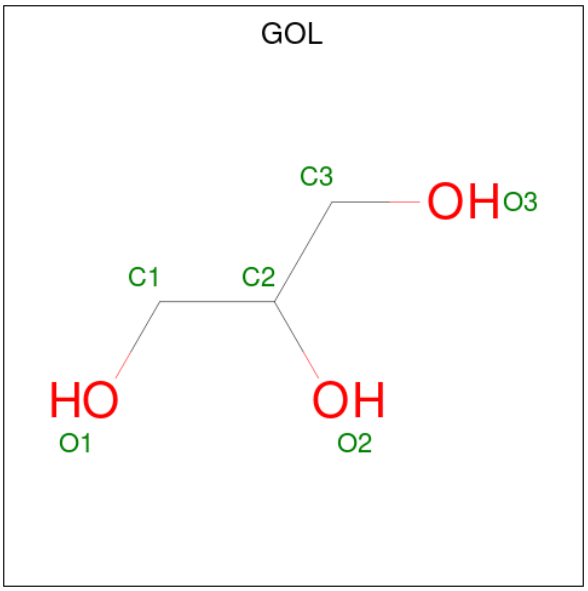
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	LEU	-	expression tag	UNP O18423
A	299	VAL	-	expression tag	UNP O18423
A	300	PRO	-	expression tag	UNP O18423
A	301	ARG	-	expression tag	UNP O18423
A	302	GLY	-	expression tag	UNP O18423
A	303	SER	-	expression tag	UNP O18423
A	304	GLY	-	expression tag	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

Continued on next page...

Continued from previous page...

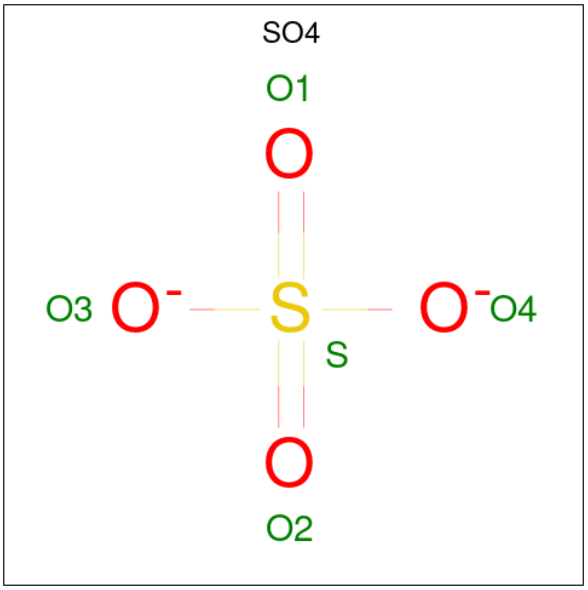
Chain	Residue	Modelled	Actual	Comment	Reference
B	306	HIS	-	expression tag	UNP O18423
B	307	HIS	-	expression tag	UNP O18423
B	308	HIS	-	expression tag	UNP O18423
B	309	HIS	-	expression tag	UNP O18423
B	310	HIS	-	expression tag	UNP O18423
C	298	LEU	-	expression tag	UNP O18423
C	299	VAL	-	expression tag	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: $C_3H_8O_3$).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

Continued on next page...

Continued from previous page...

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

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

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

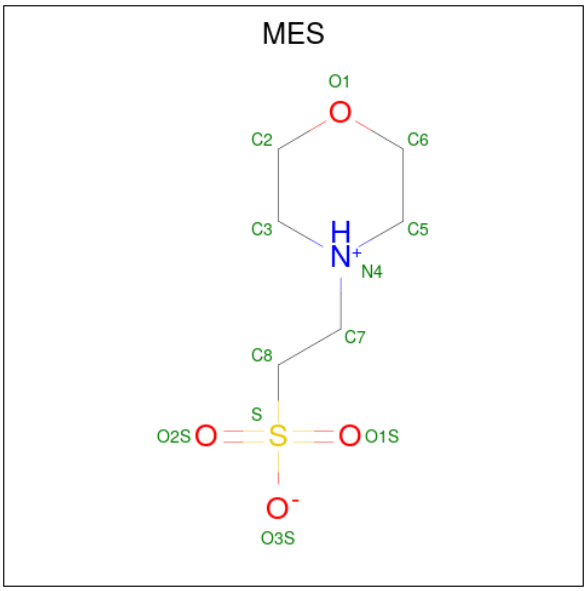
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 8 is water.

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

3 Residue-property plots (i)

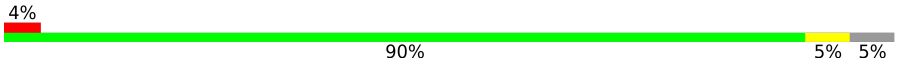
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

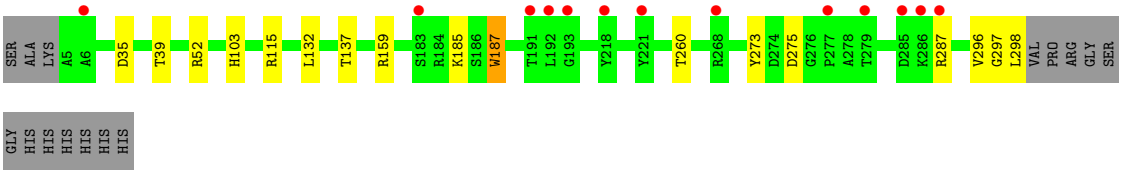
• Molecule 1: LYSENIN

Chain A:

• Molecule 1: LYSENIN

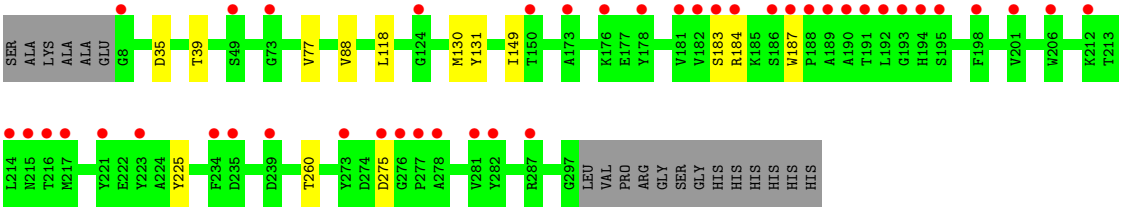
Chain B:





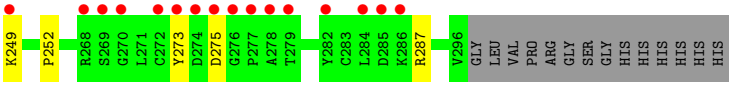
• Molecule 1: LYSENIN

Chain C:



• Molecule 1: LYSENIN

Chain D:


K249
P252
R268
S269
G270
L271
C272
Y273
D274
D275
G276
P277
A278
T279
Y282
C283
L284
D285
K286
R287
V296
GLY
LEU
VAL
PRO
ARG
GLY
SER
GLY
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

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 39.37 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.09-3.30) 97.7 (39.37-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.213 , 0.236 0.236 , 0.258	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 , 62.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, NA, MG, CL, MES, 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	0.34	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(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	291/309 (94%)	274 (94%)	16 (6%)	1 (0%)	41	71
1	B	292/309 (94%)	276 (94%)	13 (4%)	3 (1%)	15	46
1	C	288/309 (93%)	271 (94%)	14 (5%)	3 (1%)	15	46
1	D	287/309 (93%)	270 (94%)	16 (6%)	1 (0%)	41	71
All	All	1158/1236 (94%)	1091 (94%)	59 (5%)	8 (1%)	22	54

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	256/268 (96%)	248 (97%)	8 (3%)	40	67
1	B	256/268 (96%)	247 (96%)	9 (4%)	36	64
1	C	254/268 (95%)	247 (97%)	7 (3%)	43	70
1	D	254/268 (95%)	248 (98%)	6 (2%)	49	73
All	All	1020/1072 (95%)	990 (97%)	30 (3%)	42	69

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

Continued on next page...

Continued from previous page...

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	473	-	4,4,4	1.93	1 (25%)	6,6,6	0.97	1 (16%)
3	SO4	B	468	-	4,4,4	1.87	1 (25%)	6,6,6	1.00	1 (16%)
2	GOL	A	398	-	5,5,5	0.33	0	5,5,5	0.23	0
2	GOL	C	398	-	5,5,5	0.53	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	D	467	6	4,4,4	1.92	1 (25%)	6,6,6	0.95	0
7	MES	D	921	-	12,12,12	1.02	1 (8%)	14,16,16	1.17	2 (14%)
7	MES	B	921	-	12,12,12	0.81	1 (8%)	14,16,16	1.21	2 (14%)
7	MES	A	921	-	12,12,12	1.03	1 (8%)	14,16,16	1.22	2 (14%)
3	SO4	B	465	6	4,4,4	1.90	1 (25%)	6,6,6	0.97	0
3	SO4	A	468	6	4,4,4	1.86	1 (25%)	6,6,6	1.01	1 (16%)
3	SO4	A	466	-	4,4,4	1.90	1 (25%)	6,6,6	0.98	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
2	GOL	A	398	-	-	0/4/4/4	-
2	GOL	C	398	-	-	0/4/4/4	-
7	MES	D	921	-	-	5/6/14/14	0/1/1/1
7	MES	B	921	-	-	2/6/14/14	0/1/1/1
7	MES	A	921	-	-	2/6/14/14	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	473	SO4	O1-S	3.31	1.64	1.46
3	D	467	SO4	O1-S	3.29	1.63	1.46
3	A	466	SO4	O1-S	3.27	1.63	1.46
3	B	465	SO4	O1-S	3.27	1.63	1.46
7	A	921	MES	C8-S	3.26	1.82	1.77
3	B	468	SO4	O1-S	3.22	1.63	1.46
3	A	468	SO4	O1-S	3.18	1.63	1.46
7	D	921	MES	C8-S	3.17	1.82	1.77
7	B	921	MES	C8-S	2.55	1.81	1.77

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	921	MES	O1S-S-C8	2.39	109.79	106.92
7	A	921	MES	O1S-S-C8	2.28	109.66	106.92
7	B	921	MES	O3S-S-C8	2.15	109.24	105.77
7	D	921	MES	O3S-S-C8	2.13	109.21	105.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	468	SO4	O3-S-O2	2.12	120.37	109.31
7	A	921	MES	O3S-S-C8	2.11	109.19	105.77
7	B	921	MES	O1S-S-C8	2.10	109.44	106.92
3	B	468	SO4	O3-S-O2	2.09	120.22	109.31
3	A	466	SO4	O3-S-O2	2.06	120.07	109.31
3	B	473	SO4	O3-S-O2	2.04	119.95	109.31

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 (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, 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%)	0.25	12 (4%)	37	35	25, 48, 81, 94	0
1	B	294/309 (95%)	0.24	13 (4%)	34	33	22, 50, 98, 121	0
1	C	290/309 (93%)	0.78	43 (14%)	2	2	24, 85, 132, 148	0
1	D	289/309 (93%)	0.63	31 (10%)	6	5	25, 90, 126, 146	0
All	All	1166/1236 (94%)	0.47	99 (8%)	10	10	22, 61, 123, 148	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	182	VAL	5.4
1	C	186	SER	5.2
1	C	277	PRO	5.1
1	C	276	GLY	5.0
1	D	277	PRO	5.0
1	D	273	TYR	4.9
1	C	278	ALA	4.8
1	C	183	SER	4.7
1	C	282	TYR	4.1
1	C	181	VAL	4.1
1	D	268	ARG	4.1
1	C	221	TYR	4.0
1	C	234	PHE	3.7
1	A	286	LYS	3.7
1	C	275	ASP	3.6
1	D	285	ASP	3.6
1	D	286	LYS	3.6
1	C	176	LYS	3.5
1	B	279	THR	3.5
1	C	193	GLY	3.5
1	D	11	GLN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	192	LEU	3.5
1	D	269	SER	3.5
1	C	184	ARG	3.4
1	C	187	TRP	3.4
1	C	190	ALA	3.4
1	C	189	ALA	3.4
1	D	275	ASP	3.4
1	C	206	TRP	3.3
1	A	278	ALA	3.3
1	B	191	THR	3.2
1	C	217	MET	3.2
1	C	235	ASP	3.2
1	B	286	LYS	3.2
1	B	277	PRO	3.2
1	C	173	ALA	3.2
1	D	282	TYR	3.0
1	B	285	ASP	3.0
1	C	216	THR	3.0
1	C	194	HIS	2.9
1	D	8	GLY	2.9
1	C	223	TYR	2.8
1	D	276	GLY	2.8
1	C	212	LYS	2.8
1	D	31	SER	2.8
1	D	49	SER	2.7
1	C	195	SER	2.7
1	D	198	PHE	2.7
1	D	165	LYS	2.7
1	D	248	ASN	2.6
1	D	239	ASP	2.6
1	B	6	ALA	2.6
1	C	198	PHE	2.6
1	D	197	LEU	2.6
1	B	192	LEU	2.5
1	C	191	THR	2.5
1	B	183	SER	2.5
1	A	189	ALA	2.5
1	C	150	THR	2.5
1	C	239	ASP	2.4
1	D	175	ARG	2.4
1	B	221	TYR	2.4
1	D	194	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	72	ILE	2.4
1	D	270	GLY	2.4
1	A	50	GLU	2.4
1	C	214	LEU	2.4
1	C	49	SER	2.4
1	C	8	GLY	2.3
1	C	201	VAL	2.3
1	A	48	ASN	2.3
1	B	218	TYR	2.3
1	C	188	PRO	2.3
1	C	287	ARG	2.3
1	D	183	SER	2.3
1	C	178	TYR	2.3
1	C	124	GLY	2.3
1	D	272	CYS	2.3
1	A	277	PRO	2.3
1	D	284	LEU	2.2
1	D	249	LYS	2.2
1	D	192	LEU	2.2
1	A	279	THR	2.2
1	D	279	THR	2.2
1	C	273	TYR	2.2
1	D	278	ALA	2.1
1	C	73	GLY	2.1
1	D	274	ASP	2.1
1	A	216	THR	2.1
1	A	49	SER	2.1
1	C	215	ASN	2.1
1	A	159	ARG	2.1
1	B	193	GLY	2.1
1	B	287	ARG	2.1
1	A	263	ASN	2.1
1	A	140	GLY	2.1
1	C	281	VAL	2.0
1	B	268	ARG	2.0
1	D	63	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.41	0.77	55,55,55,55	0
7	MES	D	921	12/12	0.65	0.32	134,138,144,146	0
2	GOL	C	398	6/6	0.74	0.39	31,41,44,45	0
3	SO4	D	467	5/5	0.78	0.31	74,78,80,81	5
4	NA	D	500	1/1	0.81	0.42	49,49,49,49	0
3	SO4	A	468	5/5	0.81	0.40	148,149,151,154	0
3	SO4	A	466	5/5	0.81	0.39	122,122,123,123	0
7	MES	A	921	12/12	0.83	0.32	58,61,67,69	0
3	SO4	B	473	5/5	0.84	0.31	72,76,76,78	5
3	SO4	B	468	5/5	0.85	0.33	114,116,117,117	0
6	MG	D	470	1/1	0.85	0.26	32,32,32,32	0
5	CL	A	469	1/1	0.86	0.28	61,61,61,61	0
6	MG	C	547	1/1	0.87	0.23	36,36,36,36	0
2	GOL	A	398	6/6	0.87	0.22	55,62,63,67	0
6	MG	B	472	1/1	0.89	0.18	30,30,30,30	0
6	MG	C	546	1/1	0.89	0.13	44,44,44,44	0
7	MES	B	921	12/12	0.90	0.21	61,64,71,73	0
3	SO4	B	465	5/5	0.92	0.20	31,34,36,40	5
4	NA	A	501	1/1	0.92	0.16	51,51,51,51	0
6	MG	B	470	1/1	0.93	0.15	27,27,27,27	0
4	NA	A	467	1/1	0.93	0.23	25,25,25,25	0
4	NA	B	500	1/1	0.94	0.23	24,24,24,24	0
4	NA	A	502	1/1	0.94	0.23	40,40,40,40	0
4	NA	A	500	1/1	0.96	0.51	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.