



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 10:08 AM EST

PDB ID : 3CQ9  
Title : Crystal structure of the lp\_1622 protein from Lactobacillus plantarum. Northeast Structural Genomics Consortium target LpR114  
Authors : Vorobiev, S.M.; Abashidze, M.; Seetharaman, J.; Zhao, L.; Maglaqui, M.; Foote, E.L.; Ciccocanti, C.; Janjua, H.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2008-04-02  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

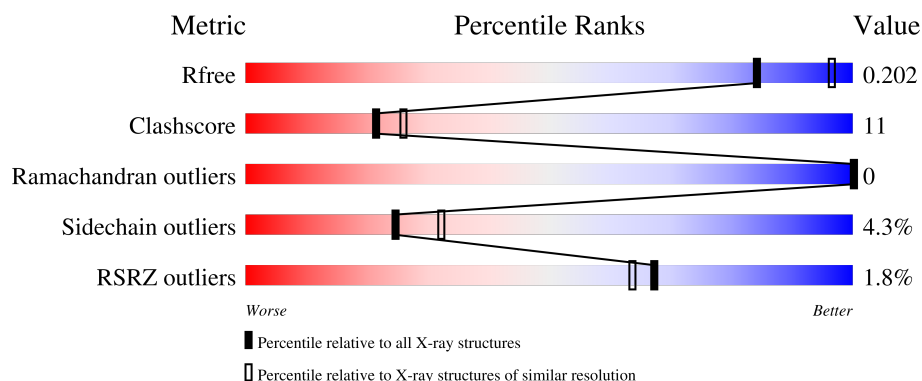
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	<div> <div>0%</div> <div>67% 21% • 11%</div> </div>
1	B	227	<div> <div>3%</div> <div>75% 20% • •</div> </div>
1	C	227	<div> <div>73% 18% • 6%</div> </div>
1	D	227	<div> <div>2%</div> <div>65% 22% • 11%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7249 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 Uncharacterized protein lp\_1622.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	Se	0	0	0
			1560	1009	264	283	4			
1	B	219	Total	C	N	O	Se	0	0	0
			1694	1088	284	317	5			
1	C	213	Total	C	N	O	Se	0	0	0
			1656	1067	279	306	4			
1	D	203	Total	C	N	O	Se	0	0	0
			1578	1020	267	287	4			

There are 32 discrepancies between the modelled and reference sequences:

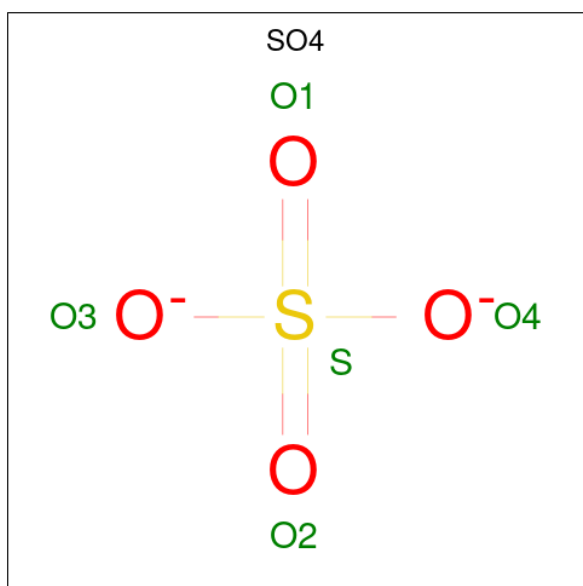
Chain	Residue	Modelled	Actual	Comment	Reference
A	220	LEU	-	expression tag	UNP Q88WK7
A	221	GLU	-	expression tag	UNP Q88WK7
A	222	HIS	-	expression tag	UNP Q88WK7
A	223	HIS	-	expression tag	UNP Q88WK7
A	224	HIS	-	expression tag	UNP Q88WK7
A	225	HIS	-	expression tag	UNP Q88WK7
A	226	HIS	-	expression tag	UNP Q88WK7
A	227	HIS	-	expression tag	UNP Q88WK7
B	220	LEU	-	expression tag	UNP Q88WK7
B	221	GLU	-	expression tag	UNP Q88WK7
B	222	HIS	-	expression tag	UNP Q88WK7
B	223	HIS	-	expression tag	UNP Q88WK7
B	224	HIS	-	expression tag	UNP Q88WK7
B	225	HIS	-	expression tag	UNP Q88WK7
B	226	HIS	-	expression tag	UNP Q88WK7
B	227	HIS	-	expression tag	UNP Q88WK7
C	220	LEU	-	expression tag	UNP Q88WK7
C	221	GLU	-	expression tag	UNP Q88WK7
C	222	HIS	-	expression tag	UNP Q88WK7
C	223	HIS	-	expression tag	UNP Q88WK7
C	224	HIS	-	expression tag	UNP Q88WK7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	225	HIS	-	expression tag	UNP Q88WK7
C	226	HIS	-	expression tag	UNP Q88WK7
C	227	HIS	-	expression tag	UNP Q88WK7
D	220	LEU	-	expression tag	UNP Q88WK7
D	221	GLU	-	expression tag	UNP Q88WK7
D	222	HIS	-	expression tag	UNP Q88WK7
D	223	HIS	-	expression tag	UNP Q88WK7
D	224	HIS	-	expression tag	UNP Q88WK7
D	225	HIS	-	expression tag	UNP Q88WK7
D	226	HIS	-	expression tag	UNP Q88WK7
D	227	HIS	-	expression tag	UNP Q88WK7

- 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	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		

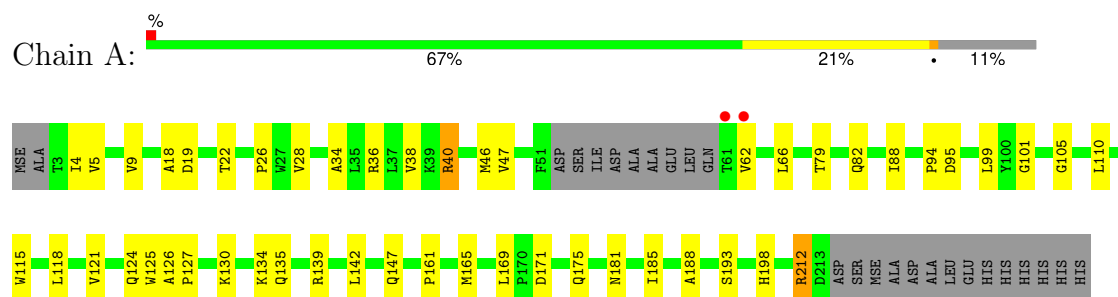
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	172	Total 172	O 172	0	0
3	B	191	Total 191	O 191	0	0
3	C	222	Total 222	O 222	0	0
3	D	156	Total 156	O 156	0	0

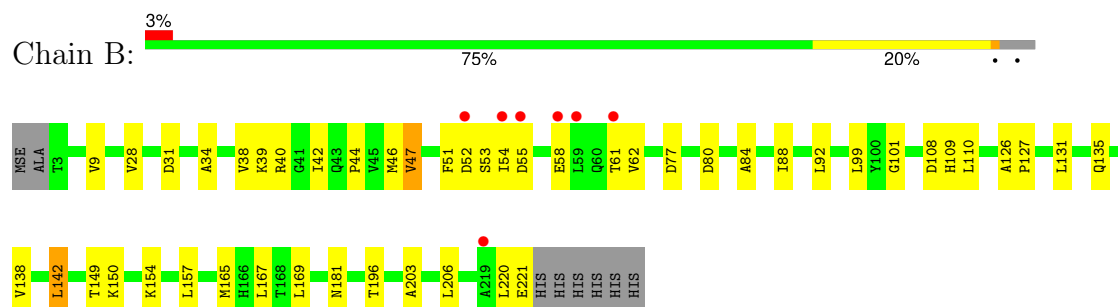
### 3 Residue-property plots [i](#)

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.

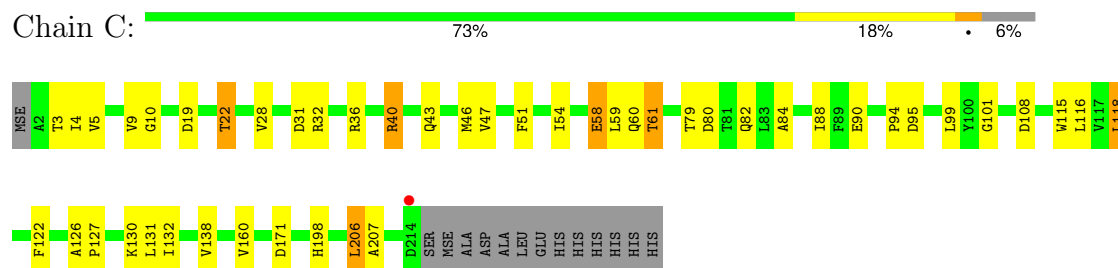
#### • Molecule 1: Uncharacterized protein lp\_1622



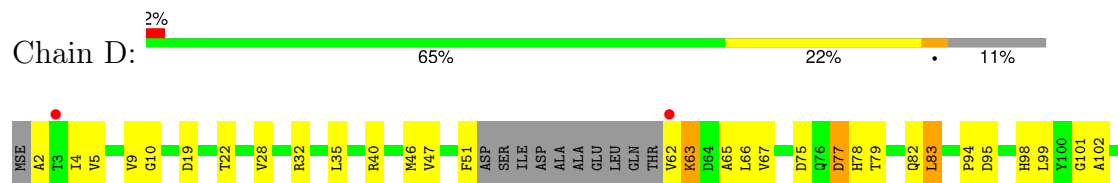
#### • Molecule 1: Uncharacterized protein lp\_1622



#### • Molecule 1: Uncharacterized protein lp\_1622



#### • Molecule 1: Uncharacterized protein lp\_1622





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.78Å 194.03Å 52.09Å 90.00° 115.34° 90.00°	Depositor
Resolution (Å)	44.67 – 2.20 44.67 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.0 (44.67-2.20) 97.0 (44.67-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.08 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.181 , 0.204 0.183 , 0.202	Depositor DCC
$R_{free}$ test set	2182 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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	0.34	0/1597	0.66	1/2176 (0.0%)
1	B	0.33	0/1731	0.68	0/2357
1	C	0.33	0/1694	0.69	2/2307 (0.1%)
1	D	0.33	0/1615	0.65	1/2199 (0.0%)
All	All	0.33	0/6637	0.67	4/9039 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	LEU	CA-CB-CG	5.36	127.64	115.30
1	C	10	GLY	N-CA-C	5.26	126.25	113.10
1	A	193	SER	N-CA-C	-5.19	96.99	111.00
1	D	10	GLY	N-CA-C	5.04	125.70	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	1560	0	1526	35	0
1	B	1694	0	1662	29	0
1	C	1656	0	1637	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1578	0	1557	45	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	10	0	0	0	0
3	A	172	0	0	3	0
3	B	191	0	0	1	0
3	C	222	0	0	4	0
3	D	156	0	0	1	0
All	All	7249	0	6382	138	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 11.

All (138) 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:54:ILE:HD11	1:C:59:LEU:HA	1.44	0.99
1:D:195:ASN:H	1:D:195:ASN:HD22	1.08	0.98
1:C:3:THR:HG23	1:C:95:ASP:H	1.31	0.95
1:D:195:ASN:H	1:D:195:ASN:ND2	1.61	0.94
1:A:46:MSE:HE1	1:A:88:ILE:HG13	1.49	0.93
1:D:195:ASN:HD22	1:D:195:ASN:N	1.68	0.91
1:A:28:VAL:HG11	1:A:46:MSE:HE2	1.53	0.91
1:A:36:ARG:O	1:A:40:ARG:HD2	1.76	0.86
1:A:28:VAL:HG11	1:A:46:MSE:CE	2.09	0.81
1:C:36:ARG:O	1:C:40:ARG:HD2	1.80	0.81
1:C:54:ILE:HD11	1:C:59:LEU:CA	2.19	0.72
1:D:63:LYS:HD2	1:D:66:LEU:HD22	1.72	0.71
1:D:47:VAL:HG12	1:D:51:PHE:CE2	2.28	0.68
1:A:147:GLN:HE21	1:A:198:HIS:HE1	1.40	0.67
1:C:84:ALA:O	1:C:88:ILE:HG13	1.96	0.66
1:A:18:ALA:HB2	3:A:1049:HOH:O	1.97	0.65
1:C:115:TRP:HB3	1:C:118:LEU:HD22	1.78	0.65
1:B:46:MSE:HE2	1:B:92:LEU:HD11	1.79	0.65
1:C:19:ASP:O	1:C:22:THR:HB	1.97	0.64
1:C:171:ASP:OD2	1:C:198:HIS:HD2	1.81	0.63
1:C:126:ALA:HB3	1:C:127:PRO:HD3	1.81	0.63
1:D:165:MSE:HG2	1:D:181:ASN:HD21	1.63	0.62
1:D:62:VAL:HG12	1:D:63:LYS:HD3	1.82	0.62
1:D:79:THR:OG1	1:D:82:GLN:HG3	2.00	0.62
1:D:19:ASP:O	1:D:22:THR:HB	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:CG1	1:A:46:MSE:HE2	2.27	0.60
1:D:99:LEU:HD23	1:D:131:LEU:CD2	2.32	0.60
1:C:3:THR:HG23	1:C:95:ASP:N	2.10	0.60
1:C:60:GLN:HG2	3:C:936:HOH:O	2.01	0.60
1:B:165:MSE:HG2	1:B:181:ASN:HD21	1.67	0.59
1:A:130:LYS:HD3	1:A:139:ARG:HG2	1.83	0.59
1:D:62:VAL:O	1:D:65:ALA:HB3	2.04	0.58
1:A:19:ASP:O	1:A:22:THR:HB	2.04	0.57
1:D:161:PRO:HG2	1:D:185:ILE:HG22	1.86	0.57
1:D:28:VAL:HG22	1:D:46:MSE:HB3	1.86	0.57
1:B:9:VAL:HG23	1:B:101:GLY:O	2.03	0.57
1:B:84:ALA:O	1:B:88:ILE:HG13	2.05	0.56
1:D:2:ALA:N	1:D:95:ASP:OD2	2.37	0.56
1:D:99:LEU:HD23	1:D:131:LEU:HD22	1.86	0.56
1:D:32:ARG:NH2	3:D:1112:HOH:O	2.39	0.56
1:A:110:LEU:C	1:A:110:LEU:HD23	2.26	0.55
1:B:47:VAL:HG13	1:B:51:PHE:CE2	2.41	0.55
1:D:157:LEU:O	1:D:190:ASN:HB3	2.05	0.55
1:D:75:ASP:HB2	1:D:83:LEU:HG	1.89	0.55
1:A:121:VAL:HG11	3:A:680:HOH:O	2.07	0.54
1:C:82:GLN:HB3	1:C:122:PHE:CZ	2.43	0.54
1:B:220:LEU:O	1:B:221:GLU:CB	2.56	0.53
1:A:46:MSE:CE	1:A:88:ILE:HG13	2.30	0.53
1:D:212:ARG:NH1	1:D:213:ASP:O	2.42	0.53
3:A:761:HOH:O	1:B:109:HIS:HE1	1.92	0.53
1:A:9:VAL:HG23	1:A:101:GLY:O	2.09	0.53
1:C:58:GLU:O	1:C:61:THR:HG23	2.09	0.53
1:C:3:THR:HG22	1:C:95:ASP:CG	2.29	0.53
1:A:169:LEU:O	1:A:175:GLN:HB3	2.09	0.53
1:D:133:ASP:OD1	1:D:136:ASN:N	2.41	0.52
1:A:126:ALA:HB3	1:A:127:PRO:HD3	1.90	0.52
1:A:79:THR:OG1	1:A:82:GLN:HG3	2.09	0.52
1:D:115:TRP:HB3	1:D:118:LEU:HD12	1.92	0.51
1:C:47:VAL:CG1	1:C:51:PHE:CE2	2.94	0.50
1:D:99:LEU:HG	1:D:102:ALA:HB2	1.91	0.50
1:B:131:LEU:HB3	1:B:138:VAL:HB	1.93	0.50
1:B:46:MSE:HE1	1:B:88:ILE:HG12	1.93	0.50
1:B:149:THR:HG22	1:B:196:THR:HG22	1.92	0.50
1:C:31:ASP:OD1	1:C:80:ASP:OD2	2.30	0.49
1:A:4:ILE:O	1:A:26:PRO:HD2	2.12	0.49
1:A:147:GLN:HE21	1:A:198:HIS:CE1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:ASN:ND2	1:D:195:ASN:N	2.31	0.49
1:A:5:VAL:HG23	1:A:94:PRO:HB3	1.94	0.49
1:C:131:LEU:HB2	1:C:138:VAL:HB	1.94	0.49
1:D:51:PHE:O	1:D:63:LYS:HE3	2.13	0.48
1:B:28:VAL:HG21	1:B:46:MSE:HE3	1.94	0.48
1:C:130:LYS:HE3	1:C:132:ILE:HD11	1.94	0.48
1:D:9:VAL:HG23	1:D:101:GLY:O	2.13	0.48
1:D:126:ALA:HB3	1:D:127:PRO:HD3	1.95	0.48
1:A:115:TRP:HB3	1:A:118:LEU:HD12	1.94	0.48
1:A:134:LYS:O	1:A:212:ARG:NH1	2.47	0.48
1:B:47:VAL:HG13	1:B:51:PHE:HE2	1.77	0.48
1:D:5:VAL:HG23	1:D:94:PRO:HB3	1.96	0.48
1:D:165:MSE:HE2	1:D:203:ALA:O	2.14	0.48
1:C:40:ARG:NH1	3:C:421:HOH:O	2.46	0.47
1:B:126:ALA:HB3	1:B:127:PRO:HD3	1.96	0.47
1:C:3:THR:HG22	1:C:95:ASP:OD2	2.14	0.47
1:A:188:ALA:HB2	1:B:108:ASP:HB2	1.97	0.47
1:A:130:LYS:HD3	1:A:139:ARG:CG	2.45	0.46
1:A:105:GLY:HA2	1:B:135:GLN:NE2	2.30	0.46
1:A:34:ALA:O	1:A:38:VAL:HG23	2.16	0.46
1:A:62:VAL:O	1:A:66:LEU:HD13	2.16	0.46
1:B:150:LYS:HE2	1:B:154:LYS:O	2.15	0.46
1:B:167:LEU:HG	1:B:169:LEU:HD13	1.96	0.46
1:D:160:VAL:HB	1:D:207:ALA:HB3	1.96	0.46
1:C:79:THR:OG1	1:C:82:GLN:HG3	2.16	0.46
1:B:28:VAL:CG2	1:B:46:MSE:HE3	2.46	0.46
1:C:5:VAL:HG23	1:C:94:PRO:HB3	1.97	0.46
1:C:90:GLU:HB3	3:C:748:HOH:O	2.15	0.45
1:C:160:VAL:HB	1:C:207:ALA:HB3	1.98	0.45
1:D:161:PRO:HB3	1:D:165:MSE:SE	2.67	0.45
1:C:9:VAL:HG23	1:C:101:GLY:O	2.16	0.45
1:A:124:GLN:HG2	1:A:125:TRP:N	2.32	0.45
1:C:32:ARG:NH2	1:C:36:ARG:HH22	2.15	0.45
1:A:161:PRO:HD2	1:A:185:ILE:O	2.18	0.44
1:B:58:GLU:O	1:B:62:VAL:HG23	2.16	0.44
1:C:54:ILE:HD12	1:C:54:ILE:C	2.37	0.44
1:D:110:LEU:C	1:D:110:LEU:HD23	2.38	0.44
1:B:53:SER:HB3	3:B:771:HOH:O	2.18	0.44
1:B:42:ILE:O	1:B:44:PRO:HD3	2.17	0.44
1:D:126:ALA:N	1:D:127:PRO:CD	2.81	0.44
1:D:161:PRO:HG2	1:D:185:ILE:CG2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LEU:HB2	1:D:138:VAL:HB	1.99	0.44
1:A:171:ASP:OD2	1:A:198:HIS:CD2	2.71	0.43
1:D:124:GLN:H	1:D:124:GLN:HG3	1.47	0.43
1:C:3:THR:CG2	1:C:95:ASP:H	2.17	0.43
1:B:110:LEU:C	1:B:110:LEU:HD23	2.38	0.43
1:D:47:VAL:CG1	1:D:51:PHE:CE2	2.97	0.43
1:C:108:ASP:HB2	1:D:188:ALA:HB2	2.01	0.42
1:B:31:ASP:OD1	1:B:80:ASP:OD2	2.37	0.42
1:A:165:MSE:HG2	1:A:181:ASN:HD21	1.85	0.42
1:B:52:ASP:OD1	1:B:53:SER:N	2.53	0.42
1:D:35:LEU:HD22	1:D:35:LEU:H	1.84	0.42
1:C:28:VAL:HG22	1:C:46:MSE:HB3	2.02	0.42
1:C:126:ALA:N	1:C:127:PRO:CD	2.82	0.42
1:B:40:ARG:HH11	1:B:40:ARG:HG3	1.85	0.42
1:C:43:GLN:HG3	3:C:1027:HOH:O	2.18	0.42
1:B:34:ALA:O	1:B:38:VAL:HG23	2.20	0.42
1:C:32:ARG:NH2	1:C:36:ARG:NH2	2.67	0.42
1:D:4:ILE:HD13	1:D:98:HIS:CE1	2.54	0.42
1:A:134:LYS:HG3	1:A:135:GLN:HG3	2.02	0.41
1:D:75:ASP:HB3	1:D:78:HIS:HB2	2.01	0.41
1:A:95:ASP:OD2	1:D:2:ALA:N	2.54	0.41
1:B:39:LYS:HE3	2:B:303:SO4:O4	2.20	0.41
1:B:165:MSE:HE2	1:B:203:ALA:O	2.20	0.41
1:A:47:VAL:HG21	1:A:66:LEU:HG	2.03	0.41
1:D:63:LYS:O	1:D:67:VAL:HG23	2.20	0.41
1:D:190:ASN:OD1	1:D:191:GLU:N	2.48	0.41
1:D:35:LEU:HD22	1:D:35:LEU:N	2.36	0.41
1:D:75:ASP:OD1	1:D:77:ASP:N	2.54	0.41
1:A:28:VAL:CG1	1:A:46:MSE:CE	2.91	0.41
1:B:142:LEU:HD12	1:B:142:LEU:HA	1.89	0.40
1:A:28:VAL:HG11	1:A:46:MSE:HE3	1.97	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	198/227 (87%)	195 (98%)	3 (2%)	0	100	100
1	B	217/227 (96%)	212 (98%)	5 (2%)	0	100	100
1	C	211/227 (93%)	208 (99%)	3 (1%)	0	100	100
1	D	199/227 (88%)	197 (99%)	2 (1%)	0	100	100
All	All	825/908 (91%)	812 (98%)	13 (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	162/183 (88%)	158 (98%)	4 (2%)	42	56
1	B	179/183 (98%)	170 (95%)	9 (5%)	20	26
1	C	175/183 (96%)	166 (95%)	9 (5%)	20	25
1	D	166/183 (91%)	159 (96%)	7 (4%)	25	33
All	All	682/732 (93%)	653 (96%)	29 (4%)	25	32

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	99	LEU
1	A	142	LEU
1	A	212	ARG
1	B	47	VAL
1	B	54	ILE
1	B	55	ASP
1	B	61	THR
1	B	77	ASP
1	B	99	LEU

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Mol	Chain	Res	Type
1	B	142	LEU
1	B	157	LEU
1	B	206	LEU
1	C	4	ILE
1	C	22	THR
1	C	40	ARG
1	C	58	GLU
1	C	61	THR
1	C	99	LEU
1	C	116	LEU
1	C	118	LEU
1	C	206	LEU
1	D	40	ARG
1	D	63	LYS
1	D	77	ASP
1	D	83	LEU
1	D	124	GLN
1	D	157	LEU
1	D	195	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	91	GLN
1	A	93	GLN
1	A	109	HIS
1	A	113	ASN
1	A	135	GLN
1	A	175	GLN
1	A	181	ASN
1	A	198	HIS
1	B	91	GLN
1	B	135	GLN
1	B	175	GLN
1	B	181	ASN
1	C	43	GLN
1	C	135	GLN
1	C	175	GLN
1	C	198	HIS
1	D	15	ASN
1	D	76	GLN

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Mol	Chain	Res	Type
1	D	93	GLN
1	D	109	HIS
1	D	147	GLN
1	D	181	ASN
1	D	195	ASN
1	D	198	HIS

### 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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	304	-	4,4,4	0.39	0	6,6,6	0.06	0
2	SO4	C	301	-	4,4,4	0.33	0	6,6,6	0.06	0
2	SO4	B	303	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	C	302	-	4,4,4	0.32	0	6,6,6	0.09	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	303	SO4	1	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, 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	198/227 (87%)	-0.29	2 (1%) 79 76	12, 20, 34, 41	0
1	B	214/227 (94%)	-0.23	7 (3%) 49 46	9, 19, 43, 51	0
1	C	209/227 (92%)	-0.47	1 (0%) 87 85	8, 18, 28, 38	0
1	D	199/227 (87%)	-0.07	5 (2%) 58 55	13, 22, 42, 55	0
All	All	820/908 (90%)	-0.27	15 (1%) 67 64	8, 20, 38, 55	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	VAL	3.4
1	B	52	ASP	3.4
1	D	195	ASN	3.3
1	B	61	THR	3.1
1	D	174	TYR	2.9
1	B	58	GLU	2.9
1	A	62	VAL	2.8
1	C	214	ASP	2.8
1	D	194	GLY	2.8
1	A	61	THR	2.6
1	D	3	THR	2.6
1	B	54	ILE	2.5
1	B	55	ASP	2.5
1	B	59	LEU	2.1
1	B	219	ALA	2.1

### 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, 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	A	304	5/5	0.92	0.11	27,34,37,39	0
2	SO4	B	303	5/5	0.95	0.09	30,31,33,40	0
2	SO4	C	302	5/5	0.96	0.09	34,38,41,44	0
2	SO4	C	301	5/5	0.99	0.09	24,24,29,29	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.