



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:08 pm GMT

PDB ID : 1LUR  
Title : Crystal Structure of the GalM/aldose Epimerase Homologue from *C. elegans*,  
Northeast Structural Genomics Target WR66  
Authors : Keller, J.P.; Xiao, R.; MacDonald, L.; Shen, J.; Acton, T.; Montelione, G.;  
Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2002-05-23  
Resolution : 1.85 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

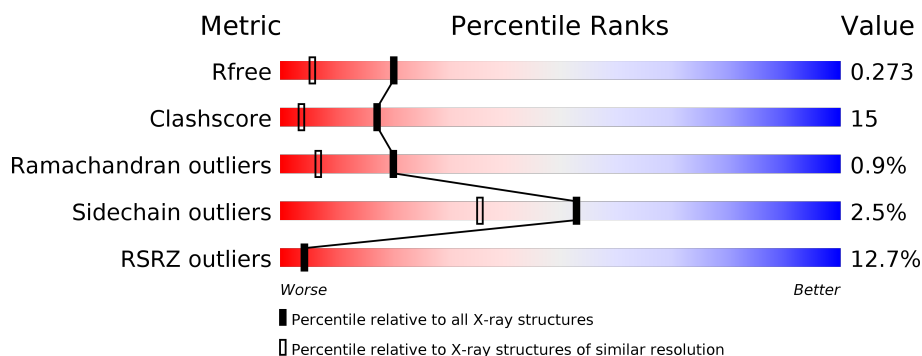
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	100719	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

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	339	
1	B	339	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5504 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 aldose 1-epimerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	Se	50	0	0
			2548	1610	433	499	4	2			
1	B	325	Total	C	N	O	S	Se	0	0	0
			2548	1610	433	499	4	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	992	MSE	-	EXPRESSION TAG	UNP Q966D4
A	993	SER	-	EXPRESSION TAG	UNP Q966D4
A	994	HIS	-	EXPRESSION TAG	UNP Q966D4
A	995	HIS	-	EXPRESSION TAG	UNP Q966D4
A	996	HIS	-	EXPRESSION TAG	UNP Q966D4
A	997	HIS	-	EXPRESSION TAG	UNP Q966D4
A	998	HIS	-	EXPRESSION TAG	UNP Q966D4
A	999	HIS	-	EXPRESSION TAG	UNP Q966D4
A	1000	SER	-	EXPRESSION TAG	UNP Q966D4
A	1001	MSE	MET	MODIFIED RESIDUE	UNP Q966D4
A	1082	MSE	MET	MODIFIED RESIDUE	UNP Q966D4
A	1181	MSE	MET	MODIFIED RESIDUE	UNP Q966D4
B	1992	MSE	-	EXPRESSION TAG	UNP Q966D4
B	1993	SER	-	EXPRESSION TAG	UNP Q966D4
B	1994	HIS	-	EXPRESSION TAG	UNP Q966D4
B	1995	HIS	-	EXPRESSION TAG	UNP Q966D4
B	1996	HIS	-	EXPRESSION TAG	UNP Q966D4
B	1997	HIS	-	EXPRESSION TAG	UNP Q966D4
B	1998	HIS	-	EXPRESSION TAG	UNP Q966D4
B	1999	HIS	-	EXPRESSION TAG	UNP Q966D4
B	2000	SER	-	EXPRESSION TAG	UNP Q966D4
B	2001	MSE	MET	MODIFIED RESIDUE	UNP Q966D4
B	2082	MSE	MET	MODIFIED RESIDUE	UNP Q966D4
B	2181	MSE	MET	MODIFIED RESIDUE	UNP Q966D4

- 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		

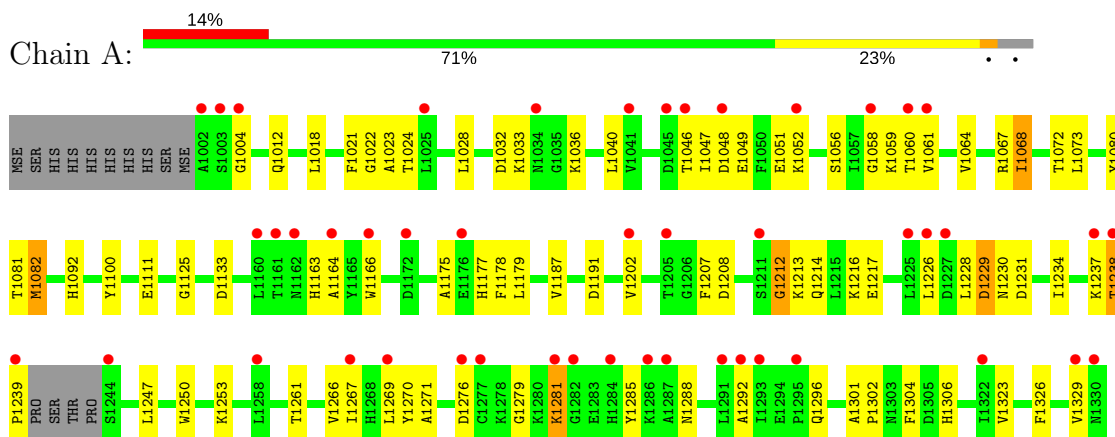
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	162	Total	O	0	0
			162	162		
3	B	236	Total	O	0	0
			236	236		

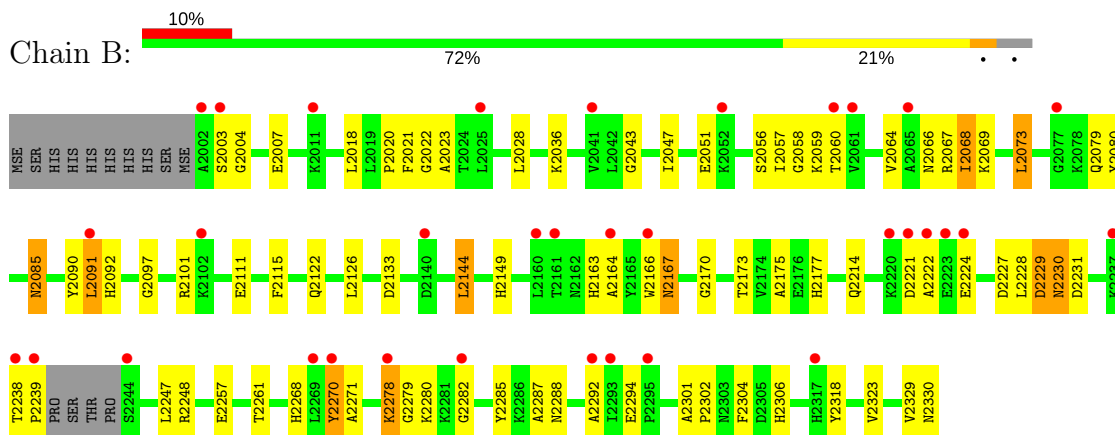
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: aldose 1-epimerase



#### • Molecule 1: aldose 1-epimerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.81Å 91.01Å 83.70Å 90.00° 100.67° 90.00°	Depositor
Resolution (Å)	20.00 – 1.85 32.59 – 1.84	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-1.85) 93.7 (32.59-1.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.262 0.230 , 0.273	Depositor DCC
$R_{free}$ test set	3005 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5504	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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	0.33	0/2608	0.66	3/3535 (0.1%)
1	B	0.35	0/2608	0.72	3/3535 (0.1%)
All	All	0.34	0/5216	0.69	6/7070 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2060	THR	N-CA-C	-6.04	94.68	111.00
1	A	1060	THR	N-CA-C	-5.69	95.64	111.00
1	B	2068	ILE	N-CA-C	-5.58	95.92	111.00
1	A	1068	ILE	N-CA-C	-5.53	96.06	111.00
1	A	1067	ARG	N-CA-C	5.30	125.31	111.00
1	B	2144	LEU	N-CA-C	-5.29	96.72	111.00

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	2548	0	2440	61	0
1	B	2548	0	2440	93	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
3	A	162	0	0	3	0
3	B	236	0	0	6	0
All	All	5504	0	4880	153	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 15.

All (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2278:LYS:HD3	1:B:2282:GLY:HA2	1.39	1.02
1:B:2067:ARG:HH12	1:B:2091:LEU:HD12	1.24	1.00
1:B:2085:ASN:HD21	1:B:2091:LEU:H	0.99	0.93
1:B:2268:HIS:HB3	1:B:2294:GLU:HG3	1.54	0.89
1:A:1238:THR:H	1:A:1239:PRO:HD2	1.42	0.85
1:B:2270:TYR:N	1:B:2270:TYR:HD2	1.75	0.85
1:A:1080:TYR:HB3	1:A:1082:MSE:HE1	1.61	0.83
1:A:1082:MSE:HE2	1:A:1125:GLY:O	1.83	0.78
1:B:2067:ARG:HH11	1:B:2067:ARG:HG2	1.47	0.78
1:B:2270:TYR:N	1:B:2270:TYR:CD2	2.50	0.77
1:B:2003:SER:HB3	1:B:2020:PRO:HG2	1.69	0.75
1:B:2066:ASN:HD22	1:B:2067:ARG:H	1.34	0.74
1:B:2091:LEU:O	1:B:2091:LEU:HD23	1.89	0.72
1:B:2085:ASN:ND2	1:B:2091:LEU:H	1.81	0.72
1:B:2066:ASN:H	1:B:2092:HIS:HD2	1.36	0.71
1:B:2270:TYR:CE2	1:B:2292:ALA:HB3	2.27	0.70
1:A:1279:GLY:HA3	1:A:1285:TYR:CE2	2.28	0.69
1:B:2101:ARG:HH11	1:B:2101:ARG:HB3	1.58	0.69
1:A:1175:ALA:HB1	1:A:1216:LYS:HB3	1.74	0.69
1:B:2101:ARG:HB3	1:B:2101:ARG:NH1	2.08	0.68
1:A:1187:VAL:HB	1:A:1231:ASP:HB2	1.75	0.66
1:B:2067:ARG:NH1	1:B:2091:LEU:HD12	2.04	0.66
1:B:2066:ASN:H	1:B:2092:HIS:CD2	2.13	0.66
1:B:2085:ASN:HD21	1:B:2091:LEU:N	1.84	0.65
1:A:1228:LEU:HB3	1:A:1271:ALA:HB2	1.79	0.64
1:B:2229:ASP:H	1:B:2230:ASN:HD22	1.45	0.64
1:A:1081:THR:C	1:A:1082:MSE:HE3	2.18	0.64
1:A:1072:THR:HG23	1:A:1081:THR:HG22	1.79	0.64
1:B:2163:HIS:CD2	1:B:2270:TYR:HH	2.16	0.63
1:A:1046:THR:OG1	1:A:1049:GLU:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:ASP:OD1	1:A:1052:LYS:HE3	2.00	0.62
1:B:2167:ASN:ND2	1:B:2170:GLY:H	1.97	0.62
1:A:1261:THR:HG22	1:A:1323:VAL:HB	1.80	0.61
1:B:2091:LEU:C	1:B:2091:LEU:HD23	2.21	0.61
1:B:2270:TYR:HE2	1:B:2294:GLU:HG2	1.65	0.61
1:B:2069:LYS:HE2	3:B:3095:HOH:O	2.00	0.61
1:A:1270:TYR:HB3	1:A:1292:ALA:HB3	1.83	0.60
1:B:2066:ASN:ND2	1:B:2067:ARG:H	2.00	0.59
1:A:1238:THR:N	1:A:1239:PRO:HD2	2.17	0.59
1:A:1018:LEU:HD22	1:A:1018:LEU:N	2.18	0.58
1:A:1238:THR:H	1:A:1239:PRO:CD	2.16	0.57
1:B:2238:THR:N	1:B:2239:PRO:HD2	2.20	0.57
1:B:2270:TYR:CE2	1:B:2294:GLU:HG2	2.39	0.57
1:A:1213:LYS:HD2	1:A:1217:GLU:HB2	1.87	0.56
1:A:1271:ALA:O	1:A:1288:ASN:HA	2.05	0.56
1:B:2073:LEU:HD21	1:B:2080:TYR:HB2	1.86	0.56
1:B:2270:TYR:CZ	1:B:2294:GLU:CD	2.78	0.56
1:A:1021:PHE:CE2	1:A:1051:GLU:HA	2.41	0.56
1:A:1056:SER:O	1:A:1163:HIS:HB3	2.06	0.56
1:B:2270:TYR:OH	1:B:2294:GLU:OE1	2.24	0.55
1:A:1266:VAL:HG22	1:A:1296:GLN:O	2.06	0.55
1:B:2270:TYR:CD2	1:B:2292:ALA:HB3	2.42	0.55
1:B:2163:HIS:CE1	1:B:2270:TYR:CE1	2.94	0.55
1:A:1081:THR:O	1:A:1082:MSE:HE3	2.07	0.54
1:B:2018:LEU:HD22	1:B:2018:LEU:N	2.23	0.54
1:B:2028:LEU:HD12	1:B:2144:LEU:HD22	1.90	0.54
1:B:2004:GLY:HA2	1:B:2047:ILE:CD1	2.36	0.54
1:A:1004:GLY:HA2	1:A:1047:ILE:HD11	1.90	0.54
1:B:2073:LEU:HD23	1:B:2073:LEU:N	2.24	0.53
1:B:2228:LEU:O	1:B:2270:TYR:HA	2.09	0.53
1:B:2073:LEU:N	1:B:2073:LEU:CD2	2.72	0.53
1:B:2268:HIS:CD2	1:B:2294:GLU:OE2	2.61	0.53
1:A:1046:THR:HB	3:A:3016:HOH:O	2.09	0.53
1:A:1247:LEU:HD23	1:A:1247:LEU:C	2.29	0.53
1:B:2043:GLY:HA3	1:B:2280:LYS:HE3	1.90	0.53
1:B:2247:LEU:HD23	1:B:2247:LEU:C	2.30	0.53
1:B:2004:GLY:HA2	1:B:2047:ILE:HD11	1.90	0.52
1:B:2067:ARG:HH11	1:B:2067:ARG:CG	2.15	0.52
1:B:2021:PHE:CE2	1:B:2051:GLU:HA	2.44	0.52
1:B:2085:ASN:HD22	1:B:2085:ASN:H	1.57	0.52
1:A:1032:ASP:OD2	1:A:1036:LYS:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1229:ASP:H	1:A:1230:ASN:HD22	1.58	0.51
1:B:2270:TYR:OH	1:B:2294:GLU:CD	2.49	0.51
1:B:2231:ASP:HA	1:B:2268:HIS:HA	1.93	0.51
1:B:2064:VAL:HG11	1:B:2068:ILE:HD11	1.92	0.51
1:A:1281:LYS:HA	1:A:1281:LYS:HE3	1.93	0.51
1:B:2270:TYR:CE2	1:B:2292:ALA:CB	2.93	0.51
1:B:2073:LEU:CD2	1:B:2080:TYR:HB2	2.40	0.51
1:B:2270:TYR:H	1:B:2270:TYR:HD2	1.58	0.50
1:A:1028:LEU:HD22	1:A:1040:LEU:HD12	1.94	0.50
1:B:2271:ALA:O	1:B:2288:ASN:HA	2.11	0.50
1:B:2067:ARG:NH1	1:B:2067:ARG:CG	2.75	0.49
1:A:1279:GLY:HA3	1:A:1285:TYR:CZ	2.47	0.49
1:A:1304:PHE:HB3	1:A:1306:HIS:CE1	2.47	0.49
1:A:1028:LEU:HD13	1:A:1166:TRP:CH2	2.48	0.49
1:B:2133:ASP:OD1	1:B:2149:HIS:HB3	2.13	0.49
1:B:2227:ASP:HB2	3:B:3331:HOH:O	2.12	0.48
1:B:2163:HIS:CE1	1:B:2270:TYR:HE1	2.32	0.48
1:B:2278:LYS:CD	1:B:2282:GLY:HA2	2.28	0.48
1:A:1028:LEU:HD11	1:A:1326:PHE:CZ	2.49	0.48
1:B:2090:TYR:HE2	1:B:2126:LEU:HD21	1.79	0.48
1:B:2028:LEU:HD13	1:B:2166:TRP:CH2	2.48	0.48
1:A:1226:LEU:H	1:A:1288:ASN:HD21	1.62	0.47
1:A:1179:LEU:O	1:A:1212:GLY:HA2	2.15	0.47
1:B:2097:GLY:O	1:B:2101:ARG:HG2	2.13	0.47
1:A:1033:LYS:HE2	1:A:1253:LYS:O	2.15	0.47
1:B:2043:GLY:CA	1:B:2280:LYS:HE3	2.43	0.47
1:A:1329:VAL:O	1:A:1329:VAL:HG13	2.15	0.47
1:B:2073:LEU:HD23	1:B:2073:LEU:H	1.80	0.46
1:A:1177:HIS:O	1:A:1214:GLN:HA	2.14	0.46
1:B:2028:LEU:HD13	1:B:2166:TRP:HH2	1.80	0.46
1:B:2007:GLU:HB3	3:B:3236:HOH:O	2.15	0.46
1:B:2248:ARG:HD2	1:B:2257:GLU:OE2	2.17	0.45
1:A:1301:ALA:N	1:A:1302:PRO:CD	2.80	0.45
1:B:2173:THR:HG23	1:B:2175:ALA:H	1.80	0.45
1:B:2221:ASP:OD1	1:B:2224:GLU:HB3	2.17	0.45
1:B:2229:ASP:H	1:B:2230:ASN:ND2	2.13	0.45
1:A:1072:THR:HG23	1:A:1081:THR:CG2	2.46	0.45
1:A:1064:VAL:HG11	1:A:1068:ILE:HD11	1.99	0.44
1:A:1056:SER:HA	1:A:1059:LYS:HD2	1.99	0.44
1:B:2301:ALA:N	1:B:2302:PRO:CD	2.80	0.44
1:A:1208:ASP:O	1:A:1213:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:LYS:N	1:A:1237:LYS:HD2	2.32	0.44
1:A:1058:GLY:HA2	1:A:1164:ALA:HA	1.99	0.44
1:B:2173:THR:HG21	3:B:3274:HOH:O	2.17	0.44
1:B:2058:GLY:HA2	1:B:2164:ALA:HA	1.99	0.43
1:B:2287:ALA:O	1:B:2288:ASN:HB2	2.18	0.43
1:A:1028:LEU:HD13	1:A:1166:TRP:CZ3	2.53	0.43
1:B:2056:SER:HA	1:B:2059:LYS:HD2	1.99	0.43
1:B:2028:LEU:CD1	1:B:2144:LEU:HD22	2.49	0.43
1:B:2149:HIS:HA	1:B:2318:TYR:O	2.18	0.43
1:B:2133:ASP:OD2	1:B:2149:HIS:HD2	2.02	0.43
1:B:2304:PHE:HB3	1:B:2306:HIS:CE1	2.54	0.43
1:B:2115:PHE:O	1:B:2133:ASP:HA	2.18	0.43
1:B:2279:GLY:HA3	1:B:2285:TYR:CZ	2.54	0.43
1:B:2261:THR:HG22	1:B:2323:VAL:HB	2.00	0.43
1:B:2079:GLN:HG3	3:B:3209:HOH:O	2.19	0.43
1:B:2085:ASN:N	1:B:2085:ASN:HD22	2.15	0.43
1:B:2279:GLY:HA3	1:B:2285:TYR:CE1	2.54	0.43
1:A:1100:TYR:HE2	3:A:3151:HOH:O	2.02	0.42
1:A:1080:TYR:CB	1:A:1082:MSE:HE1	2.43	0.42
1:A:1226:LEU:H	1:A:1288:ASN:ND2	2.18	0.42
1:A:1229:ASP:HA	1:A:1269:LEU:O	2.19	0.42
1:A:1073:LEU:C	1:A:1073:LEU:HD12	2.39	0.42
1:A:1261:THR:CG2	1:A:1323:VAL:HB	2.47	0.42
1:B:2057:ILE:HG22	3:B:3122:HOH:O	2.17	0.42
1:A:1022:GLY:O	1:A:1023:ALA:C	2.58	0.42
1:A:1061:VAL:HG13	1:A:1092:HIS:HB3	2.01	0.42
1:B:2163:HIS:NE2	1:B:2270:TYR:HE1	2.18	0.42
1:A:1271:ALA:HB3	3:A:3054:HOH:O	2.20	0.41
1:B:2167:ASN:HD22	1:B:2167:ASN:C	2.24	0.41
1:B:2270:TYR:CZ	1:B:2292:ALA:CB	3.04	0.41
1:A:1024:THR:HG23	1:A:1058:GLY:C	2.41	0.41
1:A:1202:VAL:CG2	1:A:1207:PHE:C	2.89	0.41
1:B:2329:VAL:O	1:B:2330:ASN:HB2	2.20	0.41
1:B:2022:GLY:O	1:B:2023:ALA:C	2.59	0.41
1:B:2067:ARG:NH1	1:B:2067:ARG:HG2	2.25	0.41
1:B:2177:HIS:O	1:B:2214:GLN:HA	2.21	0.41
1:A:1012:GLN:HA	1:B:2036:LYS:HB2	2.03	0.40
1:A:1234:ILE:HD11	1:A:1267:ILE:HG13	2.03	0.40
1:B:2167:ASN:HD21	1:B:2170:GLY:H	1.70	0.40
1:A:1178:PHE:HB2	1:A:1250:TRP:CE2	2.57	0.40
1:A:1238:THR:N	1:A:1239:PRO:CD	2.80	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	321/339 (95%)	302 (94%)	15 (5%)	4 (1%)	15	4
1	B	321/339 (95%)	304 (95%)	15 (5%)	2 (1%)	28	13
All	All	642/678 (95%)	606 (94%)	30 (5%)	6 (1%)	20	7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1229	ASP
1	B	2222	ALA
1	A	1212	GLY
1	A	1238	THR
1	A	1276	ASP
1	B	2229	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	276/286 (96%)	271 (98%)	5 (2%)	64	50
1	B	276/286 (96%)	267 (97%)	9 (3%)	43	24
All	All	552/572 (96%)	538 (98%)	14 (2%)	53	35

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1082	MSE
1	A	1111	GLU
1	A	1133	ASP
1	A	1191	ASP
1	A	1281	LYS
1	B	2073	LEU
1	B	2085	ASN
1	B	2091	LEU
1	B	2111	GLU
1	B	2122	GLN
1	B	2167	ASN
1	B	2230	ASN
1	B	2270	TYR
1	B	2278	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1037	ASN
1	A	1079	GLN
1	A	1149	HIS
1	A	1230	ASN
1	A	1288	ASN
1	A	1317	HIS
1	B	2012	GLN
1	B	2038	GLN
1	B	2066	ASN
1	B	2070	ASN
1	B	2079	GLN
1	B	2085	ASN
1	B	2086	ASN
1	B	2092	HIS
1	B	2096	ASN
1	B	2122	GLN
1	B	2149	HIS
1	B	2167	ASN
1	B	2230	ASN
1	B	2317	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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	4001	-	4,4,4	0.36	0	6,6,6	0.06	0
2	SO4	B	4002	-	4,4,4	0.33	0	6,6,6	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	4001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	4002	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	316/339 (93%)	0.82	47 (14%) <b>3</b> <b>3</b>	20, 35, 57, 71	0
1	B	323/339 (95%)	0.61	34 (10%) <b>7</b> <b>7</b>	18, 28, 46, 68	0
All	All	639/678 (94%)	0.71	81 (12%) <b>4</b> <b>4</b>	18, 31, 56, 71	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1239	PRO	10.8
1	B	2002	ALA	10.4
1	A	1238	THR	10.3
1	A	1002	ALA	9.2
1	B	2239	PRO	8.9
1	B	2238	THR	8.4
1	B	2222	ALA	7.5
1	B	2220	LYS	7.4
1	A	1003	SER	7.1
1	B	2237	LYS	7.1
1	B	2270	TYR	6.8
1	B	2223	GLU	5.9
1	B	2221	ASP	5.7
1	A	1330	ASN	5.7
1	A	1237	LYS	5.1
1	A	1293	ILE	4.6
1	A	1269	LEU	4.4
1	A	1282	GLY	4.4
1	A	1286	LYS	4.4
1	B	2003	SER	4.3
1	B	2011	LYS	3.9
1	A	1281	LYS	3.9
1	A	1164	ALA	3.5
1	A	1291	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	2052	LYS	3.3
1	B	2160	LEU	3.3
1	A	1284	HIS	3.3
1	A	1292	ALA	3.2
1	A	1244	SER	3.2
1	A	1061	VAL	3.2
1	A	1258	LEU	3.1
1	A	1161	THR	3.1
1	A	1267	ILE	3.1
1	A	1176	GLU	3.1
1	B	2061	VAL	3.0
1	B	2292	ALA	3.0
1	A	1172	ASP	2.9
1	A	1046	THR	2.8
1	A	1211	SER	2.8
1	B	2091	LEU	2.8
1	A	1226	LEU	2.8
1	B	2025	LEU	2.7
1	B	2166	TRP	2.7
1	B	2244	SER	2.7
1	A	1160	LEU	2.7
1	A	1041	VAL	2.6
1	B	2140	ASP	2.6
1	B	2164	ALA	2.6
1	A	1276	ASP	2.6
1	A	1227	ASP	2.5
1	A	1277	CYS	2.5
1	B	2293	ILE	2.5
1	A	1225	LEU	2.5
1	B	2282	GLY	2.5
1	B	2278	LYS	2.5
1	B	2224	GLU	2.5
1	A	1060	THR	2.5
1	A	1295	PRO	2.4
1	B	2060	THR	2.4
1	B	2161	THR	2.4
1	A	1004	GLY	2.4
1	A	1025	LEU	2.3
1	A	1052	LYS	2.3
1	A	1287	ALA	2.3
1	B	2269	LEU	2.3
1	A	1048	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1162	ASN	2.3
1	A	1166	TRP	2.2
1	A	1322	ILE	2.2
1	B	2317	HIS	2.2
1	B	2077	GLY	2.2
1	A	1202	VAL	2.2
1	A	1329	VAL	2.1
1	B	2295	PRO	2.1
1	B	2102	LYS	2.1
1	B	2041	VAL	2.1
1	B	2065	ALA	2.1
1	A	1045	ASP	2.1
1	A	1058	GLY	2.0
1	A	1034	ASN	2.0
1	A	1205	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 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	4002	5/5	0.98	0.11	-0.24	44,45,46,47	0
2	SO4	A	4001	5/5	0.96	0.25	-	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.