



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:33 pm BST

PDB ID : 3PQA  
Title : Crystal structure of glyceraldehyde-3-phosphate dehydrogenase GapN from Methanocaldococcus jannaschii DSM 2661  
Authors : Malashkevich, V.N.; Toro, R.; Seidel, R.; Garrett, S.; Foti, R.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2010-11-25  
Resolution : 1.50 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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

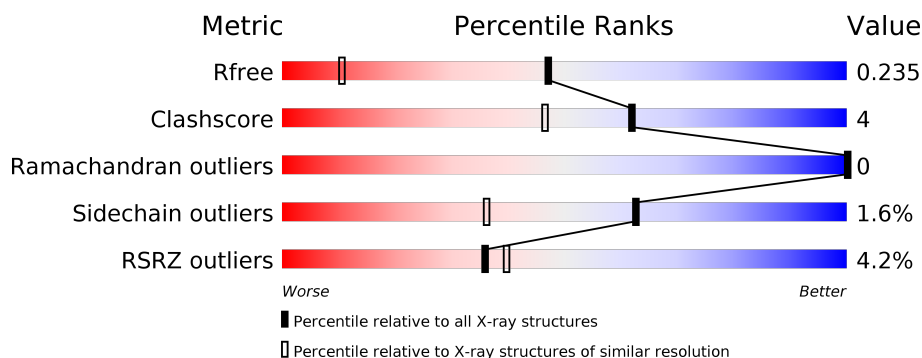
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 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	486	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	486	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	C	486	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>
1	D	486	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15744 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 Lactaldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	10	0
			3593	2308	597	673	15			
1	B	458	Total	C	N	O	S	0	10	0
			3613	2322	601	676	14			
1	C	455	Total	C	N	O	S	0	8	0
			3574	2297	596	667	14			
1	D	456	Total	C	N	O	S	0	7	0
			3574	2295	594	670	15			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	EXPRESSION TAG	UNP Q58806
A	465	ALA	-	EXPRESSION TAG	UNP Q58806
A	466	GLU	-	EXPRESSION TAG	UNP Q58806
A	467	ASN	-	EXPRESSION TAG	UNP Q58806
A	468	LEU	-	EXPRESSION TAG	UNP Q58806
A	469	TYR	-	EXPRESSION TAG	UNP Q58806
A	470	PHE	-	EXPRESSION TAG	UNP Q58806
A	471	GLN	-	EXPRESSION TAG	UNP Q58806
A	472	SER	-	EXPRESSION TAG	UNP Q58806
A	473	HIS	-	EXPRESSION TAG	UNP Q58806
A	474	HIS	-	EXPRESSION TAG	UNP Q58806
A	475	HIS	-	EXPRESSION TAG	UNP Q58806
A	476	HIS	-	EXPRESSION TAG	UNP Q58806
A	477	HIS	-	EXPRESSION TAG	UNP Q58806
A	478	HIS	-	EXPRESSION TAG	UNP Q58806
A	479	TRP	-	EXPRESSION TAG	UNP Q58806
A	480	SER	-	EXPRESSION TAG	UNP Q58806
A	481	HIS	-	EXPRESSION TAG	UNP Q58806
A	482	PRO	-	EXPRESSION TAG	UNP Q58806
A	483	GLN	-	EXPRESSION TAG	UNP Q58806
A	484	PHE	-	EXPRESSION TAG	UNP Q58806

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Chain	Residue	Modelled	Actual	Comment	Reference
A	485	GLU	-	EXPRESSION TAG	UNP Q58806
A	486	LYS	-	EXPRESSION TAG	UNP Q58806
B	1	VAL	-	EXPRESSION TAG	UNP Q58806
B	465	ALA	-	EXPRESSION TAG	UNP Q58806
B	466	GLU	-	EXPRESSION TAG	UNP Q58806
B	467	ASN	-	EXPRESSION TAG	UNP Q58806
B	468	LEU	-	EXPRESSION TAG	UNP Q58806
B	469	TYR	-	EXPRESSION TAG	UNP Q58806
B	470	PHE	-	EXPRESSION TAG	UNP Q58806
B	471	GLN	-	EXPRESSION TAG	UNP Q58806
B	472	SER	-	EXPRESSION TAG	UNP Q58806
B	473	HIS	-	EXPRESSION TAG	UNP Q58806
B	474	HIS	-	EXPRESSION TAG	UNP Q58806
B	475	HIS	-	EXPRESSION TAG	UNP Q58806
B	476	HIS	-	EXPRESSION TAG	UNP Q58806
B	477	HIS	-	EXPRESSION TAG	UNP Q58806
B	478	HIS	-	EXPRESSION TAG	UNP Q58806
B	479	TRP	-	EXPRESSION TAG	UNP Q58806
B	480	SER	-	EXPRESSION TAG	UNP Q58806
B	481	HIS	-	EXPRESSION TAG	UNP Q58806
B	482	PRO	-	EXPRESSION TAG	UNP Q58806
B	483	GLN	-	EXPRESSION TAG	UNP Q58806
B	484	PHE	-	EXPRESSION TAG	UNP Q58806
B	485	GLU	-	EXPRESSION TAG	UNP Q58806
B	486	LYS	-	EXPRESSION TAG	UNP Q58806
C	1	VAL	-	EXPRESSION TAG	UNP Q58806
C	465	ALA	-	EXPRESSION TAG	UNP Q58806
C	466	GLU	-	EXPRESSION TAG	UNP Q58806
C	467	ASN	-	EXPRESSION TAG	UNP Q58806
C	468	LEU	-	EXPRESSION TAG	UNP Q58806
C	469	TYR	-	EXPRESSION TAG	UNP Q58806
C	470	PHE	-	EXPRESSION TAG	UNP Q58806
C	471	GLN	-	EXPRESSION TAG	UNP Q58806
C	472	SER	-	EXPRESSION TAG	UNP Q58806
C	473	HIS	-	EXPRESSION TAG	UNP Q58806
C	474	HIS	-	EXPRESSION TAG	UNP Q58806
C	475	HIS	-	EXPRESSION TAG	UNP Q58806
C	476	HIS	-	EXPRESSION TAG	UNP Q58806
C	477	HIS	-	EXPRESSION TAG	UNP Q58806
C	478	HIS	-	EXPRESSION TAG	UNP Q58806
C	479	TRP	-	EXPRESSION TAG	UNP Q58806
C	480	SER	-	EXPRESSION TAG	UNP Q58806

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Chain	Residue	Modelled	Actual	Comment	Reference
C	481	HIS	-	EXPRESSION TAG	UNP Q58806
C	482	PRO	-	EXPRESSION TAG	UNP Q58806
C	483	GLN	-	EXPRESSION TAG	UNP Q58806
C	484	PHE	-	EXPRESSION TAG	UNP Q58806
C	485	GLU	-	EXPRESSION TAG	UNP Q58806
C	486	LYS	-	EXPRESSION TAG	UNP Q58806
D	1	VAL	-	EXPRESSION TAG	UNP Q58806
D	465	ALA	-	EXPRESSION TAG	UNP Q58806
D	466	GLU	-	EXPRESSION TAG	UNP Q58806
D	467	ASN	-	EXPRESSION TAG	UNP Q58806
D	468	LEU	-	EXPRESSION TAG	UNP Q58806
D	469	TYR	-	EXPRESSION TAG	UNP Q58806
D	470	PHE	-	EXPRESSION TAG	UNP Q58806
D	471	GLN	-	EXPRESSION TAG	UNP Q58806
D	472	SER	-	EXPRESSION TAG	UNP Q58806
D	473	HIS	-	EXPRESSION TAG	UNP Q58806
D	474	HIS	-	EXPRESSION TAG	UNP Q58806
D	475	HIS	-	EXPRESSION TAG	UNP Q58806
D	476	HIS	-	EXPRESSION TAG	UNP Q58806
D	477	HIS	-	EXPRESSION TAG	UNP Q58806
D	478	HIS	-	EXPRESSION TAG	UNP Q58806
D	479	TRP	-	EXPRESSION TAG	UNP Q58806
D	480	SER	-	EXPRESSION TAG	UNP Q58806
D	481	HIS	-	EXPRESSION TAG	UNP Q58806
D	482	PRO	-	EXPRESSION TAG	UNP Q58806
D	483	GLN	-	EXPRESSION TAG	UNP Q58806
D	484	PHE	-	EXPRESSION TAG	UNP Q58806
D	485	GLU	-	EXPRESSION TAG	UNP Q58806
D	486	LYS	-	EXPRESSION TAG	UNP Q58806

- 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	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		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

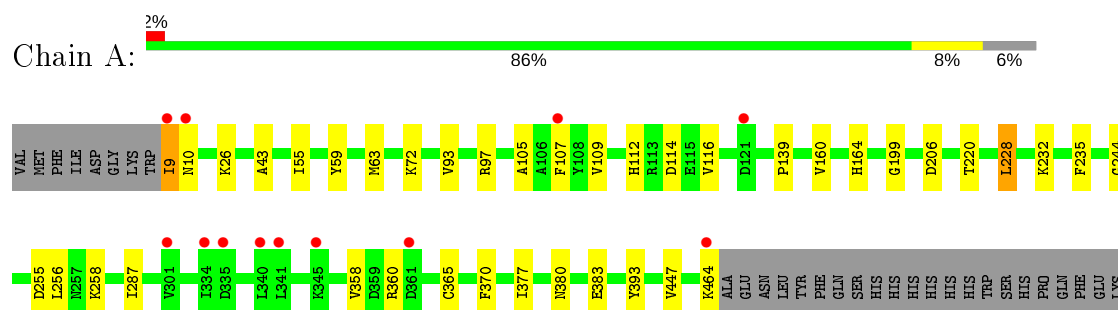
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	356	Total	O	0	0
			356	356		
3	B	354	Total	O	0	0
			354	354		
3	C	333	Total	O	0	0
			333	333		
3	D	312	Total	O	0	0
			312	312		

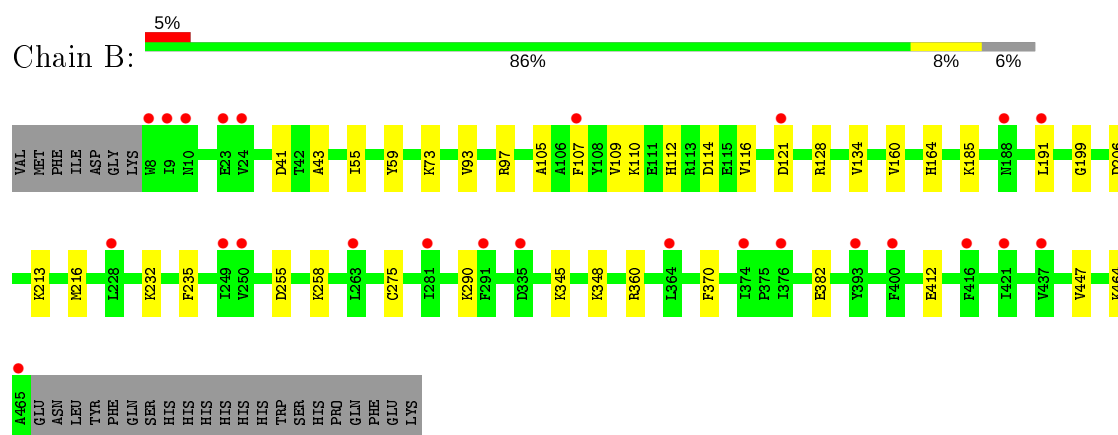
### 3 Residue-property plots [i](#)

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.

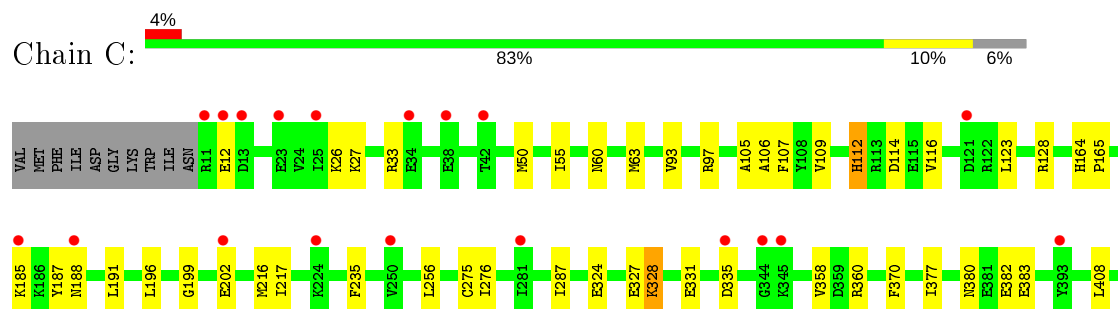
- Molecule 1: Lactaldehyde dehydrogenase

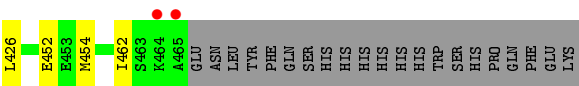


- Molecule 1: Lactaldehyde dehydrogenase

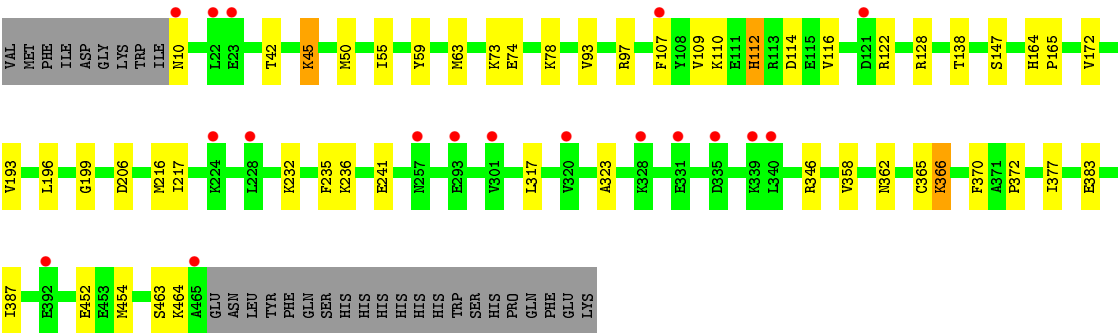
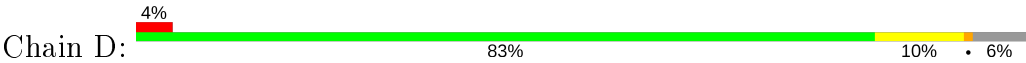


- Molecule 1: Lactaldehyde dehydrogenase





● Molecule 1: Lactaldehyde dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.57Å 77.57Å 164.28Å 90.00° 116.29° 90.00°	Depositor
Resolution (Å)	19.96 – 1.50 19.93 – 1.50	Depositor EDS
% Data completeness (in resolution range)	83.3 (19.96-1.50) 83.4 (19.93-1.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.187 , 0.222 0.203 , 0.235	Depositor DCC
$R_{free}$ test set	12500 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15744	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.81% 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	0.49	0/3678	0.60	1/4960 (0.0%)
1	B	0.48	0/3700	0.59	1/4992 (0.0%)
1	C	0.47	0/3649	0.57	0/4921
1	D	0.47	0/3649	0.57	0/4920
All	All	0.48	0/14676	0.58	2/19793 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	228	LEU	CA-CB-CG	5.05	126.92	115.30

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	3593	0	3757	27	0
1	B	3613	0	3771	31	0
1	C	3574	0	3745	49	0
1	D	3574	0	3736	34	0
2	A	10	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
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	356	0	0	3	0
3	B	354	0	0	6	0
3	C	333	0	0	9	0
3	D	312	0	0	5	0
All	All	15744	0	15009	129	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 4.

All (129) 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:128[B]:ARG:NH2	1:C:452:GLU:HG2	1.38	1.33
1:B:360[B]:ARG:HG3	1:B:360[B]:ARG:HH21	1.03	1.16
1:C:112:HIS:HD2	3:C:826:HOH:O	1.29	1.13
1:C:360[B]:ARG:HH11	1:C:360[B]:ARG:HG3	0.93	1.08
1:C:128[B]:ARG:HH22	1:C:452:GLU:CG	1.66	1.08
1:B:73:LYS:HG2	3:B:577:HOH:O	1.65	0.95
1:C:128[B]:ARG:HH22	1:C:452:GLU:HG2	0.78	0.94
1:C:360[B]:ARG:CG	1:C:360[B]:ARG:HH11	1.79	0.92
1:B:360[B]:ARG:NH2	1:B:360[B]:ARG:HG3	1.84	0.88
1:C:128[B]:ARG:NH2	1:C:452:GLU:CG	2.32	0.88
1:A:9:ILE:HA	3:A:1396:HOH:O	1.74	0.87
1:C:360[B]:ARG:HG3	1:C:360[B]:ARG:NH1	1.74	0.86
1:B:360[B]:ARG:CG	1:B:360[B]:ARG:HH21	1.89	0.85
1:B:134:VAL:HG22	1:B:216[B]:MET:HG2	1.61	0.83
1:D:216[B]:MET:HG2	1:D:217:ILE:N	1.94	0.82
1:A:72:LYS:NZ	3:A:1358:HOH:O	2.20	0.74
1:C:216[B]:MET:HG2	1:C:217:ILE:N	2.03	0.73
1:D:112:HIS:HD2	3:D:1391:HOH:O	1.72	0.72
1:A:55:ILE:HG23	1:A:109:VAL:HG12	1.71	0.72
1:B:275:CYS:SG	3:B:1223:HOH:O	2.47	0.72
1:B:412[A]:GLU:OE1	1:D:464:LYS:NZ	2.21	0.72
1:B:114[A]:ASP:HB2	1:C:116:VAL:HB	1.75	0.69
1:D:55:ILE:HG23	1:D:109:VAL:HG12	1.74	0.69
1:A:43:ALA:HB1	1:A:160:VAL:HG11	1.76	0.67
1:C:358:VAL:HG23	1:C:377:ILE:CD1	2.26	0.66
1:A:116:VAL:HB	1:D:114:ASP:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HB1	1:A:160:VAL:CG1	2.27	0.65
1:C:324:GLU:O	1:C:328:LYS:HD2	1.97	0.65
1:C:55:ILE:HG23	1:C:109[A]:VAL:HG12	1.80	0.64
1:A:107[B]:PHE:CE1	1:C:107[B]:PHE:HB3	2.34	0.63
1:C:426[A]:LEU:HG	1:C:426[A]:LEU:O	1.96	0.63
1:A:114[A]:ASP:HB2	1:D:116:VAL:HB	1.80	0.62
1:C:112:HIS:CE1	1:C:128[A]:ARG:HD2	2.34	0.62
1:A:206:ASP:OD1	1:A:232:LYS:HE2	2.00	0.62
1:C:106:ALA:O	1:C:109[B]:VAL:HG22	1.99	0.61
1:B:55:ILE:HG23	1:B:109:VAL:HG12	1.82	0.61
1:D:73:LYS:HG2	3:D:696:HOH:O	1.99	0.61
1:B:206:ASP:OD1	1:B:232:LYS:HE2	2.01	0.61
1:D:241[A]:GLU:HG2	3:D:1214:HOH:O	1.99	0.61
1:A:365:CYS:SG	1:A:377:ILE:HD11	2.42	0.60
1:C:188:ASN:HB3	3:C:576:HOH:O	2.02	0.59
1:B:275:CYS:HB3	3:B:1223:HOH:O	2.03	0.58
1:C:426[B]:LEU:HD12	1:C:426[B]:LEU:O	2.03	0.58
1:C:123:LEU:HD23	1:C:462:ILE:HD12	1.85	0.57
1:D:112:HIS:NE2	1:D:128[B]:ARG:HD2	2.20	0.57
1:D:59:TYR:CZ	1:D:63[B]:MET:SD	2.98	0.57
1:A:107[B]:PHE:CD1	1:C:107[B]:PHE:HB3	2.40	0.56
1:B:348:LYS:NZ	3:B:1161:HOH:O	2.37	0.56
1:B:116:VAL:HB	1:C:114:ASP:HB2	1.88	0.56
1:B:275:CYS:CB	3:B:1223:HOH:O	2.53	0.56
1:B:382:GLU:HG2	3:B:1071:HOH:O	2.06	0.55
1:C:105:ALA:O	1:C:109[A]:VAL:HG23	2.07	0.54
1:C:452:GLU:HG3	3:C:846:HOH:O	2.07	0.54
1:A:107[B]:PHE:CD1	1:C:107[B]:PHE:CB	2.91	0.54
1:D:358:VAL:HG23	1:D:377:ILE:CD1	2.39	0.53
1:A:112[B]:HIS:HB2	3:A:829:HOH:O	2.09	0.52
1:D:358:VAL:HG23	1:D:377:ILE:HD13	1.90	0.52
1:C:360[B]:ARG:CG	1:C:360[B]:ARG:NH1	2.50	0.52
1:B:93:VAL:O	1:B:97:ARG:HG2	2.10	0.52
1:D:323:ALA:HB1	1:D:346:ARG:HD2	1.92	0.52
1:A:358:VAL:HG23	1:A:377:ILE:HD13	1.92	0.51
1:C:12:GLU:O	1:C:27:LYS:HE3	2.10	0.51
1:A:358:VAL:HG23	1:A:377:ILE:CD1	2.40	0.51
1:D:241[A]:GLU:CG	3:D:1214:HOH:O	2.56	0.51
1:D:362:ASN:O	1:D:366:LYS:HE3	2.10	0.51
1:A:380:ASN:HB2	1:A:383:GLU:OE1	2.12	0.50
1:C:164:HIS:HE1	1:C:199:GLY:O	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:TYR:CG	1:B:110:LYS:HE3	2.48	0.49
1:A:360[B]:ARG:HH12	1:A:383:GLU:HG2	1.77	0.49
1:C:112:HIS:HB2	3:C:1269:HOH:O	2.12	0.49
1:D:164:HIS:HE1	1:D:199:GLY:O	1.96	0.49
1:D:365:CYS:SG	1:D:377:ILE:HD11	2.53	0.48
1:B:43:ALA:HB1	1:B:160:VAL:HG11	1.95	0.48
1:D:206:ASP:OD1	1:D:232:LYS:HE2	2.12	0.48
1:C:358:VAL:HG23	1:C:377:ILE:HD11	1.96	0.48
1:B:185:LYS:HE3	1:B:191:LEU:HD11	1.95	0.47
1:A:93:VAL:O	1:A:97:ARG:HG2	2.15	0.47
1:C:165:PRO:HG3	1:C:196:LEU:HD11	1.97	0.47
1:C:383:GLU:OE1	3:C:871:HOH:O	2.20	0.47
1:C:276:ILE:HG13	1:C:426[A]:LEU:HD12	1.95	0.47
1:C:128[B]:ARG:NH1	3:C:642:HOH:O	2.47	0.46
1:D:93:VAL:O	1:D:97:ARG:HG2	2.15	0.46
1:D:216[B]:MET:CE	1:D:454:MET:HG2	2.45	0.46
1:B:164:HIS:HE1	1:B:199:GLY:O	1.99	0.46
1:C:63:MET:HE3	3:C:543:HOH:O	2.16	0.46
1:C:327:GLU:O	1:C:331:GLU:HG3	2.15	0.46
1:C:112:HIS:CD2	3:C:826:HOH:O	2.20	0.46
1:B:185:LYS:HG3	1:B:191:LEU:HD21	1.98	0.45
1:D:383:GLU:HG2	1:D:387:ILE:CD1	2.47	0.45
1:C:112:HIS:HE1	1:C:128[A]:ARG:HD2	1.81	0.45
1:A:139:PRO:HD3	1:A:220:THR:HB	1.99	0.45
1:A:255:ASP:CG	1:A:258:LYS:HG3	2.37	0.45
1:B:105:ALA:HA	1:B:447:VAL:HG11	1.98	0.45
1:C:185:LYS:HG3	1:C:191:LEU:HD21	1.99	0.45
1:C:202:GLU:CD	1:C:202:GLU:H	2.21	0.45
1:C:60:ASN:HB3	1:C:187:TYR:CZ	2.52	0.45
1:C:216[B]:MET:CE	1:C:454:MET:HG2	2.46	0.44
1:B:121:ASP:HA	1:B:464:LYS:HD2	1.99	0.44
1:B:59:TYR:CD1	1:B:110:LYS:HE3	2.52	0.44
1:C:275:CYS:SG	3:C:497:HOH:O	2.61	0.44
1:C:93:VAL:O	1:C:97:ARG:HG2	2.17	0.44
1:D:74:GLU:O	1:D:78:LYS:HG2	2.17	0.44
1:C:426[A]:LEU:CG	1:C:426[A]:LEU:O	2.65	0.43
1:A:464:LYS:HE2	1:C:408:LEU:HD13	1.99	0.43
1:C:256:LEU:HD21	1:C:287:ILE:HD12	2.00	0.43
1:D:122:ARG:HG2	1:D:463:SER:HA	2.01	0.43
1:A:107[B]:PHE:CE1	1:C:107[B]:PHE:CB	3.00	0.43
1:A:164:HIS:HE1	1:A:199:GLY:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:PRO:HG3	1:D:196:LEU:HD11	2.00	0.43
1:A:105:ALA:HA	1:A:447:VAL:HG11	2.01	0.43
1:D:112:HIS:ND1	3:D:1335:HOH:O	2.33	0.43
1:B:255:ASP:CG	1:B:258:LYS:HG3	2.39	0.43
1:A:256:LEU:HD21	1:A:287:ILE:HD12	2.01	0.42
1:A:244:GLY:HA2	1:A:393:TYR:CG	2.54	0.42
1:B:41:ASP:OD1	1:B:213:LYS:HE3	2.19	0.42
1:D:452[A]:GLU:HA	1:D:452[A]:GLU:OE2	2.20	0.42
1:D:317:LEU:HD21	1:D:372:PRO:HD3	2.02	0.41
1:B:290:LYS:HB2	1:B:290:LYS:HE3	1.85	0.41
1:D:50:MET:HG2	1:D:193:VAL:CG1	2.50	0.41
1:D:217:ILE:HG12	1:D:236:LYS:HD3	2.02	0.41
1:B:107[B]:PHE:CD1	1:D:107[B]:PHE:HB3	2.55	0.41
1:D:59:TYR:CG	1:D:110:LYS:HE3	2.55	0.41
1:A:59:TYR:CZ	1:A:63[B]:MET:SD	3.13	0.41
1:B:43:ALA:HB1	1:B:160:VAL:CG1	2.51	0.41
1:D:138:THR:HG21	1:D:147:SER:HA	2.02	0.41
1:B:107[B]:PHE:CE1	1:D:107[B]:PHE:HB3	2.57	0.40
1:D:42:THR:O	1:D:45:LYS:HB2	2.22	0.40
1:C:380:ASN:ND2	1:C:382:GLU:HB2	2.37	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	464/486 (96%)	453 (98%)	11 (2%)	0	100	100
1	B	466/486 (96%)	455 (98%)	11 (2%)	0	100	100
1	C	461/486 (95%)	451 (98%)	10 (2%)	0	100	100
1	D	461/486 (95%)	450 (98%)	11 (2%)	0	100	100
All	All	1852/1944 (95%)	1809 (98%)	43 (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	399/417 (96%)	393 (98%)	6 (2%)	65	39
1	B	400/417 (96%)	395 (99%)	5 (1%)	69	44
1	C	395/417 (95%)	387 (98%)	8 (2%)	55	25
1	D	395/417 (95%)	388 (98%)	7 (2%)	59	30
All	All	1589/1668 (95%)	1563 (98%)	26 (2%)	62	36

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	10	ASN
1	A	26	LYS
1	A	228	LEU
1	A	235	PHE
1	A	370	PHE
1	B	112[A]	HIS
1	B	112[B]	HIS
1	B	235	PHE
1	B	345	LYS
1	B	370	PHE
1	C	26	LYS
1	C	33	ARG
1	C	50	MET
1	C	112	HIS
1	C	235	PHE
1	C	328	LYS
1	C	335	ASP
1	C	370	PHE
1	D	10	ASN
1	D	45	LYS
1	D	112	HIS

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Mol	Chain	Res	Type
1	D	172	VAL
1	D	235	PHE
1	D	366	LYS
1	D	370	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	257	ASN
1	B	257	ASN
1	C	112	HIS
1	C	164	HIS
1	C	322	HIS
1	C	380	ASN
1	C	405	ASN
1	D	60	ASN
1	D	164	HIS
1	D	257	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

7 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	D	488	-	4,4,4	1.86	1 (25%)	6,6,6	0.77	0
2	SO4	C	487	-	4,4,4	0.16	0	6,6,6	0.06	0
2	SO4	A	487	-	4,4,4	0.18	0	6,6,6	0.11	0
2	SO4	C	488	-	4,4,4	0.18	0	6,6,6	0.12	0
2	SO4	D	487	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	B	487	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	A	488	-	4,4,4	0.16	0	6,6,6	0.13	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	488	SO4	O2-S	-2.37	1.33	1.46

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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	456/486 (93%)	0.21	12 (2%) 56 61	8, 16, 26, 34	0
1	B	458/486 (94%)	0.41	25 (5%) 25 27	9, 16, 25, 34	0
1	C	455/486 (93%)	0.27	21 (4%) 32 35	8, 16, 25, 32	0
1	D	456/486 (93%)	0.28	18 (3%) 39 44	9, 16, 26, 35	0
All	All	1825/1944 (93%)	0.29	76 (4%) 36 40	8, 16, 26, 35	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	TRP	12.4
1	B	9	ILE	10.6
1	A	9	ILE	9.7
1	D	10	ASN	7.5
1	B	465	ALA	7.3
1	C	465	ALA	6.7
1	A	10	ASN	5.2
1	D	465	ALA	4.8
1	D	301	VAL	4.1
1	B	121	ASP	4.1
1	B	10	ASN	3.7
1	C	121	ASP	3.7
1	C	11	ARG	3.4
1	C	12	GLU	3.4
1	A	335	ASP	3.3
1	C	224	LYS	3.3
1	A	107[A]	PHE	3.2
1	D	121	ASP	3.2
1	D	320	VAL	3.2
1	A	121	ASP	3.0
1	D	340	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	42	THR	2.9
1	C	335	ASP	2.9
1	D	257	ASN	2.9
1	C	188	ASN	2.8
1	B	374	ILE	2.8
1	B	335	ASP	2.8
1	B	249	ILE	2.7
1	B	437	VAL	2.7
1	A	301	VAL	2.7
1	D	22	LEU	2.7
1	B	421	ILE	2.6
1	C	13	ASP	2.6
1	D	335	ASP	2.6
1	D	23	GLU	2.5
1	C	345	LYS	2.5
1	C	393	TYR	2.5
1	C	250	VAL	2.5
1	D	331	GLU	2.5
1	B	393	TYR	2.4
1	D	107[A]	PHE	2.4
1	C	34	GLU	2.4
1	C	23	GLU	2.4
1	B	23	GLU	2.4
1	A	340	LEU	2.4
1	B	364	LEU	2.4
1	B	376	ILE	2.3
1	D	339	LYS	2.3
1	B	228	LEU	2.3
1	B	191	LEU	2.3
1	D	224	LYS	2.3
1	B	281	ILE	2.3
1	C	281	ILE	2.3
1	C	38	GLU	2.2
1	C	464	LYS	2.2
1	D	328	LYS	2.2
1	B	188[A]	ASN	2.2
1	A	334	ILE	2.2
1	B	291	PHE	2.1
1	A	345	LYS	2.1
1	D	228	LEU	2.1
1	A	464	LYS	2.1
1	B	400	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	202	GLU	2.1
1	B	250	VAL	2.1
1	D	293	GLU	2.1
1	B	263	LEU	2.1
1	B	24	VAL	2.1
1	B	107[A]	PHE	2.1
1	C	25	ILE	2.0
1	D	392	GLU	2.0
1	A	361	ASP	2.0
1	C	185	LYS	2.0
1	B	416	PHE	2.0
1	A	341	LEU	2.0
1	C	344	GLY	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. 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	C	488	5/5	0.90	0.19	47,47,47,47	0
2	SO4	A	488	5/5	0.94	0.14	51,51,51,51	0
2	SO4	D	487	5/5	0.96	0.11	47,47,47,47	0
2	SO4	A	487	5/5	0.97	0.14	50,50,50,50	0
2	SO4	B	487	5/5	0.97	0.13	51,51,51,51	0
2	SO4	D	488	5/5	0.97	0.13	43,44,44,44	5
2	SO4	C	487	5/5	0.98	0.09	51,51,51,51	0

## 6.5 Other polymers

There are no such residues in this entry.