



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 10:08 PM GMT

PDB ID : 1F8M  
Title : CRYSTAL STRUCTURE OF 3-BROMOPYRUVATE MODIFIED ISOCITRATE LYASE (ICL) FROM MYCOBACTERIUM TUBERCULOSIS  
Authors : Sharma, V.; Sharma, S.; Hoener zu Bentrup, K.; McKinney, J.D.; Russell, D.G.; Jacobs Jr., W.R.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2000-06-30  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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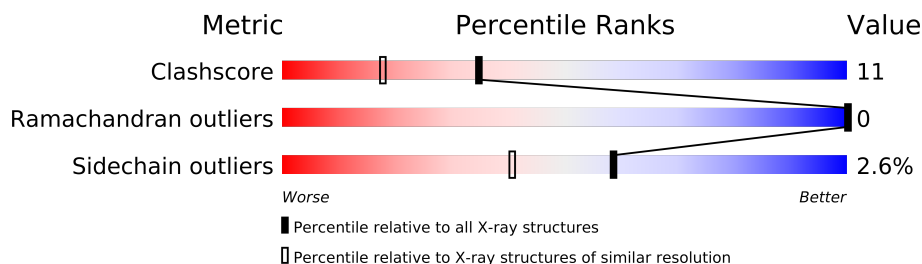
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	429	
1	B	429	
1	C	429	
1	D	429	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14276 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ISOCITRATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3308	2078	575	646	9			
1	B	427	Total	C	N	O	S	0	0	0
			3308	2078	575	646	9			
1	C	427	Total	C	N	O	S	0	0	0
			3308	2078	575	646	9			
1	D	427	Total	C	N	O	S	0	0	0
			3308	2078	575	646	9			

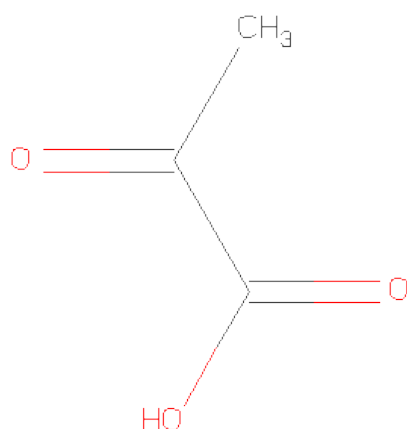
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	INSERTION	UNP P0A5H3
B	1	ALA	-	INSERTION	UNP P0A5H3
C	1	ALA	-	INSERTION	UNP P0A5H3
D	1	ALA	-	INSERTION	UNP P0A5H3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	238	Total	O	0	0
			238	238		
4	B	282	Total	O	0	0
			282	282		
4	C	272	Total	O	0	0
			272	272		
4	D	224	Total	O	0	0
			224	224		

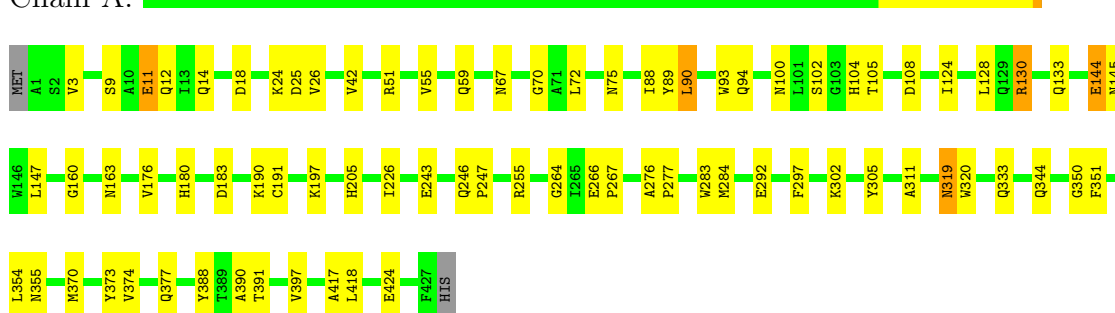
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

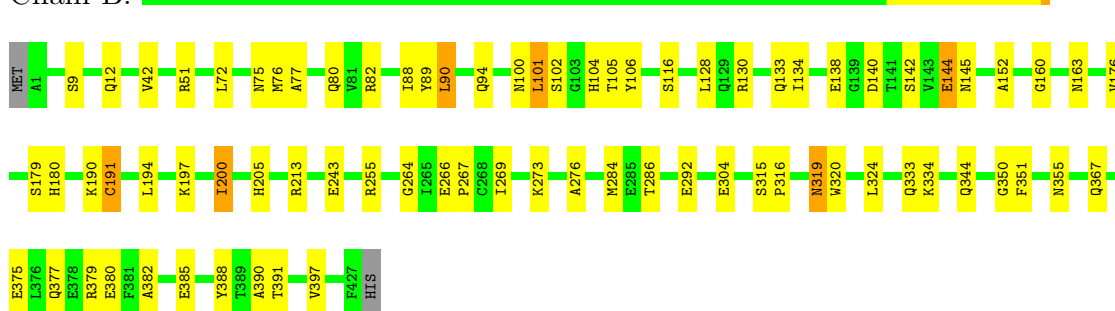
#### • Molecule 1: ISOCITRATE LYASE

Chain A:



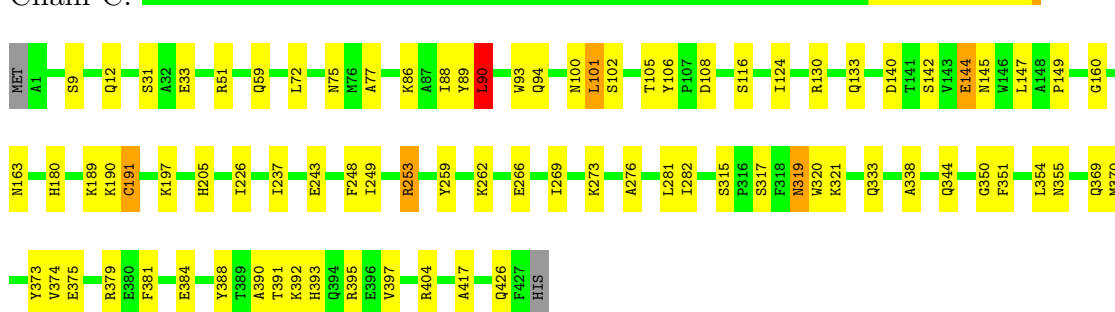
#### • Molecule 1: ISOCITRATE LYASE

Chain B:



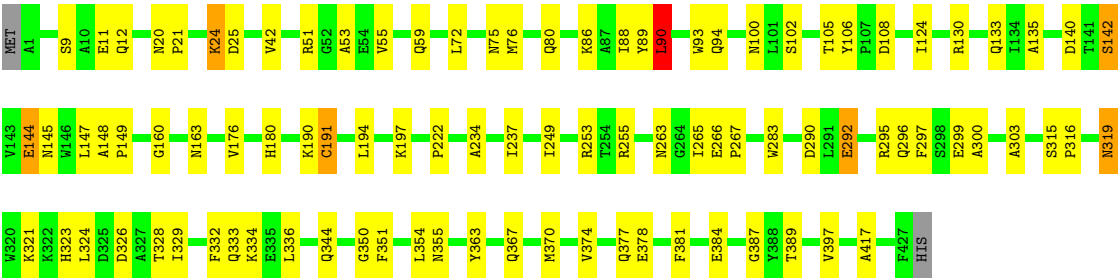
#### • Molecule 1: ISOCITRATE LYASE

Chain C:



#### • Molecule 1: ISOCITRATE LYASE

Chain D: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.31Å 129.04Å 166.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 1.80	Depositor
% Data completeness (in resolution range)	87.2 (19.86-1.80)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.203 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14276	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYR, MG

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	0.65	0/3379	0.77	3/4595 (0.1%)
1	B	0.66	0/3379	0.77	1/4595 (0.0%)
1	C	0.64	0/3379	0.76	2/4595 (0.0%)
1	D	0.62	0/3379	0.77	2/4595 (0.0%)
All	All	0.64	0/13516	0.77	8/18380 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	130	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	417	ALA	N-CA-C	5.23	125.12	111.00
1	A	183	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	90	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	417	ALA	N-CA-C	5.05	124.63	111.00
1	C	417	ALA	N-CA-C	5.03	124.58	111.00
1	D	90	LEU	CA-CB-CG	5.02	126.86	115.30

There are no chirality outliers.



All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	373	TYR	Sidechain
1	C	373	TYR	Sidechain

## 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3308	0	3192	63	0
1	B	3308	0	3192	75	0
1	C	3308	0	3192	82	0
1	D	3308	0	3192	89	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	2	1	0
3	B	6	0	2	1	0
3	C	6	0	2	0	0
3	D	6	0	2	1	0
4	A	238	0	0	5	0
4	B	282	0	0	14	0
4	C	272	0	0	10	0
4	D	224	0	0	7	0
All	All	14276	0	12776	278	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (278) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:51:ARG:HH12	1:D:145:ASN:HD21	1.07	0.99
1:B:9:SER:OG	1:B:12:GLN:HG3	1.68	0.94
1:C:130:ARG:HH11	1:C:133:GLN:HE22	1.21	0.86
1:D:51:ARG:HH12	1:D:145:ASN:ND2	1.74	0.85
1:B:77:ALA:HB1	1:B:88:ILE:HD13	1.60	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:375:GLU:O	1:C:379:ARG:HG3	1.80	0.81
1:C:253:ARG:HG3	1:C:253:ARG:HH11	1.44	0.80
1:D:265:ILE:HD13	1:D:296:GLN:HG3	1.63	0.79
1:A:264:GLY:O	1:A:267:PRO:HD2	1.83	0.78
1:A:130:ARG:HH11	1:A:133:GLN:HE22	1.31	0.77
1:A:24:LYS:HE3	1:A:25:ASP:OD2	1.87	0.75
1:B:9:SER:H	1:B:12:GLN:NE2	1.85	0.75
1:D:140:ASP:OD1	1:D:142:SER:HB3	1.89	0.73
1:C:397:VAL:HG23	1:D:105:THR:CG2	2.19	0.73
1:C:144:GLU:HG2	4:C:1572:HOH:O	1.90	0.70
1:C:397:VAL:HG23	1:D:105:THR:HG22	1.73	0.70
1:D:334:LYS:HE2	4:D:1381:HOH:O	1.92	0.69
1:A:94:GLN:HE22	1:A:350:GLY:H	1.38	0.69
1:C:130:ARG:NH1	1:C:133:GLN:HE22	1.89	0.69
1:C:144:GLU:H	1:C:144:GLU:CD	1.96	0.69
1:B:130:ARG:HH11	1:B:133:GLN:HE22	1.39	0.69
1:C:105:THR:CG2	1:D:397:VAL:HG23	2.22	0.69
1:B:292:GLU:HG3	4:B:1922:HOH:O	1.92	0.68
1:C:94:GLN:NE2	1:C:351:PHE:H	1.91	0.68
1:B:77:ALA:HB1	1:B:88:ILE:CD1	2.24	0.68
1:C:253:ARG:HD3	1:C:259:TYR:CE2	2.28	0.68
1:B:334:LYS:HE2	4:B:1977:HOH:O	1.92	0.68
1:D:144:GLU:H	1:D:144:GLU:CD	1.97	0.67
1:A:144:GLU:CD	1:A:144:GLU:H	1.98	0.67
1:A:160:GLY:H	1:A:163:ASN:HD22	1.43	0.67
1:B:255:ARG:HD3	4:B:1662:HOH:O	1.94	0.67
1:C:243:GLU:HG3	4:C:1816:HOH:O	1.93	0.66
1:D:324:LEU:HD22	1:D:328:THR:HG21	1.78	0.66
1:C:51:ARG:HH12	1:C:145:ASN:HD21	1.44	0.65
1:D:51:ARG:NH1	1:D:145:ASN:HD21	1.89	0.65
1:B:243:GLU:HG3	4:B:1805:HOH:O	1.97	0.65
1:C:140:ASP:OD1	1:C:142:SER:HB3	1.96	0.65
1:A:130:ARG:HH11	1:A:133:GLN:NE2	1.94	0.65
1:D:160:GLY:H	1:D:163:ASN:HD22	1.44	0.65
1:D:397:VAL:HG22	1:D:397:VAL:O	1.97	0.64
1:C:321:LYS:HD3	1:D:378:GLU:CD	2.17	0.64
1:C:130:ARG:HH11	1:C:133:GLN:NE2	1.94	0.64
1:C:404:ARG:NH1	4:C:1704:HOH:O	2.30	0.64
1:C:397:VAL:HG22	1:C:397:VAL:O	1.97	0.64
1:D:94:GLN:NE2	1:D:351:PHE:H	1.95	0.64
1:B:42:VAL:HG21	1:C:147:LEU:HD12	1.80	0.64
1:A:100:ASN:HD22	1:A:102:SER:H	1.46	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:160:GLY:H	1:B:163:ASN:HD22	1.46	0.63
1:A:319:ASN:HD22	1:A:319:ASN:C	2.01	0.63
1:D:90:LEU:HD22	1:D:124:ILE:HD12	1.79	0.62
1:A:418:LEU:O	1:A:424:GLU:HG3	1.99	0.62
1:C:180:HIS:HD2	4:C:1055:HOH:O	1.82	0.62
1:C:333:GLN:HA	1:C:344:GLN:HE22	1.64	0.62
1:C:253:ARG:HG3	1:C:253:ARG:NH1	2.04	0.62
1:C:189:LYS:HD3	1:C:190:LYS:N	2.14	0.62
1:B:89:TYR:OH	1:B:180:HIS:HE1	1.82	0.62
1:A:42:VAL:HG21	1:D:147:LEU:HD12	1.83	0.61
1:D:255:ARG:NH1	1:D:255:ARG:HG2	2.16	0.61
1:C:9:SER:OG	1:C:12:GLN:HG3	2.01	0.60
1:B:269:ILE:HG22	1:B:273:LYS:HE3	1.83	0.60
1:B:140:ASP:OD1	1:B:142:SER:HB3	2.01	0.60
1:C:369:GLN:OE1	1:C:369:GLN:N	2.34	0.60
1:B:51:ARG:HH12	1:B:145:ASN:HD21	1.49	0.60
1:C:105:THR:HG23	1:D:397:VAL:HG23	1.82	0.59
1:B:180:HIS:HD2	4:B:1082:HOH:O	1.84	0.59
1:A:51:ARG:HH12	1:A:145:ASN:HD21	1.50	0.59
1:D:90:LEU:CD2	1:D:124:ILE:HD12	2.33	0.59
1:C:374:VAL:HG21	1:D:329:ILE:HG21	1.84	0.59
1:D:24:LYS:HD2	1:D:25:ASP:CG	2.22	0.59
1:C:237:ILE:HG21	1:C:249:ILE:HD11	1.85	0.59
1:C:381:PHE:HA	1:C:384:GLU:OE2	2.03	0.59
3:D:500:PYR:H32	4:D:1290:HOH:O	2.02	0.58
1:B:144:GLU:CD	1:B:144:GLU:H	2.06	0.58
1:B:266:GLU:HB3	1:B:267:PRO:HD3	1.86	0.57
1:A:130:ARG:NH1	1:A:133:GLN:HE22	2.00	0.57
1:A:190:LYS:HB2	1:A:197:LYS:HG2	1.85	0.57
1:D:290:ASP:OD1	1:D:292:GLU:N	2.37	0.57
1:B:77:ALA:CB	1:B:88:ILE:HD13	2.34	0.57
1:A:255:ARG:HG3	4:A:1201:HOH:O	2.03	0.57
1:D:332:PHE:CE2	1:D:336:LEU:HD11	2.38	0.57
1:D:9:SER:OG	1:D:12:GLN:HG3	2.05	0.57
1:B:104:HIS:HE1	4:D:1481:HOH:O	1.88	0.57
1:D:255:ARG:HH11	1:D:255:ARG:HG2	1.70	0.56
1:A:105:THR:CG2	1:B:397:VAL:HG23	2.34	0.56
1:D:266:GLU:HB3	1:D:267:PRO:HD3	1.87	0.56
1:A:26:VAL:HG13	4:A:1773:HOH:O	2.05	0.56
1:C:205:HIS:HD2	4:C:1179:HOH:O	1.88	0.56
1:D:100:ASN:HD22	1:D:102:SER:H	1.51	0.56
1:C:370:MET:O	1:C:374:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:262:LYS:HG2	4:C:1953:HOH:O	2.04	0.56
1:D:354:LEU:HD23	1:D:354:LEU:C	2.25	0.56
1:B:100:ASN:HD22	1:B:102:SER:H	1.52	0.56
1:D:130:ARG:HH11	1:D:133:GLN:HE22	1.54	0.56
1:B:367:GLN:NE2	4:B:1674:HOH:O	2.39	0.56
1:A:160:GLY:H	1:A:163:ASN:ND2	2.03	0.56
1:A:105:THR:HG23	1:B:397:VAL:HG23	1.88	0.56
1:A:205:HIS:HD2	4:A:1349:HOH:O	1.89	0.55
1:B:130:ARG:HH11	1:B:133:GLN:NE2	2.03	0.55
1:A:75:ASN:HD22	1:B:355:ASN:HD21	1.54	0.55
1:A:94:GLN:HE22	1:A:350:GLY:N	2.05	0.55
1:C:248:PHE:CE1	1:C:266:GLU:HG2	2.41	0.55
1:B:130:ARG:NH1	1:B:133:GLN:HE22	2.04	0.55
1:A:333:GLN:HA	1:A:344:GLN:HE22	1.71	0.55
1:C:397:VAL:HG21	1:D:106:TYR:O	2.07	0.55
1:D:89:TYR:OH	1:D:180:HIS:HE1	1.89	0.55
1:D:295:ARG:O	1:D:299:GLU:HG3	2.07	0.55
1:B:42:VAL:HG21	1:C:147:LEU:CD1	2.37	0.55
1:D:265:ILE:HD13	1:D:296:GLN:CG	2.35	0.55
1:C:160:GLY:H	1:C:163:ASN:HD22	1.52	0.54
1:B:264:GLY:O	1:B:267:PRO:HD2	2.07	0.54
1:C:90:LEU:HD22	1:C:124:ILE:HD12	1.89	0.54
1:B:51:ARG:HH12	1:B:145:ASN:ND2	2.05	0.54
1:C:338:ALA:HB3	4:C:1781:HOH:O	2.07	0.54
1:A:388:TYR:CZ	1:A:390:ALA:HB3	2.43	0.54
3:B:500:PYR:H32	4:B:1352:HOH:O	2.06	0.54
1:A:377:GLN:HE22	1:B:320:TRP:H	1.54	0.53
1:B:205:HIS:HD2	4:B:2012:HOH:O	1.89	0.53
1:C:315:SER:OG	1:C:317:SER:HB2	2.08	0.53
1:A:264:GLY:C	1:A:267:PRO:HD2	2.29	0.53
1:C:393:HIS:O	1:C:397:VAL:HG12	2.09	0.53
1:D:180:HIS:HD2	4:D:1072:HOH:O	1.92	0.53
1:B:94:GLN:HE22	1:B:350:GLY:H	1.57	0.52
1:C:253:ARG:HD3	1:C:259:TYR:CD2	2.44	0.52
1:C:355:ASN:HD21	1:D:75:ASN:HD22	1.56	0.52
1:D:55:VAL:O	1:D:59:GLN:HG3	2.08	0.52
1:D:90:LEU:HD22	1:D:124:ILE:CD1	2.40	0.52
1:B:382:ALA:O	1:B:385:GLU:HG2	2.10	0.52
1:B:76:MET:O	1:B:80:GLN:HG3	2.10	0.52
1:A:320:TRP:H	1:B:377:GLN:HE22	1.56	0.52
1:C:100:ASN:HD22	1:C:102:SER:H	1.58	0.52
1:D:160:GLY:H	1:D:163:ASN:ND2	2.08	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:94:GLN:HE22	1:D:350:GLY:H	1.57	0.52
1:A:104:HIS:HE1	4:A:1477:HOH:O	1.93	0.52
1:A:51:ARG:HH12	1:A:145:ASN:ND2	2.08	0.52
1:C:381:PHE:CD1	1:C:391:THR:HG21	2.44	0.52
1:C:33:GLU:H	1:C:33:GLU:CD	2.14	0.51
1:C:77:ALA:HB1	1:C:88:ILE:HD13	1.92	0.51
1:B:286:THR:HG21	4:B:2008:HOH:O	2.11	0.51
1:A:88:ILE:CD1	1:A:128:LEU:HD11	2.40	0.51
1:B:333:GLN:HA	1:B:344:GLN:HE22	1.76	0.51
1:C:75:ASN:HD22	1:D:355:ASN:HD21	1.57	0.51
1:C:51:ARG:HH12	1:C:145:ASN:ND2	2.08	0.51
1:D:88:ILE:CD1	1:D:148:ALA:HB3	2.41	0.51
1:C:101:LEU:HD22	1:C:116:SER:HA	1.93	0.50
1:C:319:ASN:HD22	1:C:319:ASN:C	2.14	0.50
1:A:100:ASN:ND2	1:A:102:SER:H	2.09	0.50
1:D:253:ARG:NH1	4:D:1708:HOH:O	2.43	0.50
1:B:213:ARG:HD3	4:B:1362:HOH:O	2.12	0.50
1:C:89:TYR:OH	1:C:180:HIS:HE1	1.94	0.50
1:C:144:GLU:N	1:C:144:GLU:CD	2.65	0.50
1:C:226:ILE:HG12	1:C:281:LEU:HB2	1.93	0.50
1:A:70:GLY:HA2	1:A:89:TYR:O	2.11	0.50
1:C:106:TYR:O	1:D:397:VAL:CG2	2.60	0.49
1:C:31:SER:HB2	1:C:33:GLU:OE1	2.12	0.49
1:C:105:THR:HG22	1:D:397:VAL:HG23	1.93	0.49
1:A:130:ARG:HD3	1:A:133:GLN:NE2	2.27	0.49
1:D:190:LYS:HB2	1:D:197:LYS:HG2	1.94	0.49
1:A:266:GLU:HB3	1:A:267:PRO:HD3	1.95	0.49
1:D:237:ILE:HG21	1:D:249:ILE:HD11	1.95	0.49
1:B:269:ILE:CG2	1:B:273:LYS:HE3	2.43	0.49
1:B:94:GLN:NE2	1:B:351:PHE:H	2.10	0.49
1:D:191:CYS:HB3	1:D:194:LEU:HD12	1.94	0.49
1:A:147:LEU:HD12	1:D:42:VAL:HG21	1.94	0.49
1:B:397:VAL:HG22	1:B:397:VAL:O	2.12	0.48
1:A:67:ASN:HA	1:A:344:GLN:O	2.13	0.48
1:D:94:GLN:HE22	1:D:350:GLY:N	2.10	0.48
1:A:302:LYS:HA	1:A:305:TYR:O	2.14	0.48
1:C:276:ALA:HA	1:C:282:ILE:HD11	1.94	0.48
1:D:387:GLY:O	1:D:389:THR:HG23	2.12	0.48
1:B:134:ILE:O	1:B:138:GLU:HG3	2.13	0.48
1:D:86:LYS:O	1:D:149:PRO:HD2	2.12	0.48
1:B:89:TYR:OH	1:B:180:HIS:CE1	2.65	0.48
1:C:106:TYR:O	1:D:397:VAL:HG21	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:94:GLN:HE22	1:C:350:GLY:H	1.62	0.48
1:A:55:VAL:O	1:A:59:GLN:HG3	2.14	0.47
1:D:381:PHE:O	1:D:384:GLU:HG3	2.14	0.47
1:C:93:TRP:CD1	1:C:108:ASP:HB2	2.50	0.47
1:A:14:GLN:HG3	1:A:18:ASP:OD2	2.14	0.47
1:C:86:LYS:O	1:C:149:PRO:HD2	2.15	0.47
1:C:253:ARG:CG	1:C:253:ARG:HH11	2.18	0.47
1:A:397:VAL:HG23	1:B:105:THR:CG2	2.44	0.47
1:B:101:LEU:HD22	1:B:116:SER:HA	1.95	0.47
1:D:265:ILE:HD11	1:D:297:PHE:HB2	1.97	0.47
1:D:100:ASN:ND2	1:D:102:SER:H	2.13	0.46
1:C:108:ASP:OD2	1:C:191:CYS:HB2	2.15	0.46
1:A:354:LEU:HD23	1:A:354:LEU:C	2.36	0.46
1:C:190:LYS:HB2	1:C:197:LYS:HG2	1.96	0.46
1:B:284:MET:CE	1:B:286:THR:HG22	2.44	0.46
1:A:90:LEU:HD22	1:A:124:ILE:HD12	1.97	0.46
1:A:355:ASN:HD21	1:B:75:ASN:HD22	1.63	0.46
1:D:363:TYR:O	1:D:367:GLN:HG2	2.15	0.46
1:D:333:GLN:HA	1:D:344:GLN:HE22	1.81	0.46
1:A:397:VAL:CG2	1:B:106:TYR:O	2.64	0.46
1:C:140:ASP:OD1	1:C:142:SER:CB	2.63	0.46
1:C:392:LYS:HE3	1:C:395:ARG:HD3	1.99	0.45
1:C:397:VAL:CG2	1:D:106:TYR:O	2.64	0.45
1:A:397:VAL:HG22	1:A:397:VAL:O	2.16	0.45
1:A:94:GLN:NE2	1:A:351:PHE:H	2.13	0.45
1:C:320:TRP:H	1:D:377:GLN:HE22	1.62	0.45
1:A:93:TRP:CD1	1:A:108:ASP:HB2	2.51	0.45
1:B:380:GLU:HB3	1:B:391:THR:OG1	2.17	0.45
1:C:397:VAL:CG2	1:C:397:VAL:O	2.63	0.45
1:B:130:ARG:HD3	1:B:133:GLN:NE2	2.31	0.45
1:A:9:SER:OG	1:A:12:GLN:HG3	2.17	0.45
1:D:290:ASP:OD1	1:D:290:ASP:C	2.55	0.45
1:B:94:GLN:HE22	1:B:350:GLY:N	2.15	0.45
1:A:9:SER:OG	1:A:11:GLU:HG2	2.17	0.44
1:D:255:ARG:HH11	1:D:255:ARG:CG	2.29	0.44
1:B:191:CYS:HB3	1:B:194:LEU:HD12	1.99	0.44
1:B:276:ALA:O	4:B:1644:HOH:O	2.21	0.44
1:B:100:ASN:ND2	1:B:102:SER:H	2.16	0.44
1:D:88:ILE:HD12	1:D:148:ALA:HB3	2.00	0.44
1:D:130:ARG:HH11	1:D:133:GLN:NE2	2.13	0.43
1:D:89:TYR:OH	1:D:180:HIS:CE1	2.68	0.43
1:C:354:LEU:HD23	1:C:354:LEU:C	2.39	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:370:MET:O	1:D:374:VAL:HG23	2.18	0.43
1:D:20:ASN:HA	1:D:21:PRO:HD3	1.79	0.43
1:C:189:LYS:C	1:C:189:LYS:HD3	2.38	0.43
1:B:319:ASN:HD22	1:B:319:ASN:C	2.22	0.43
1:B:367:GLN:HG2	4:B:1674:HOH:O	2.18	0.43
1:D:93:TRP:CD1	1:D:108:ASP:HB2	2.53	0.43
1:C:426:GLN:CD	1:D:323:HIS:HE2	2.22	0.43
1:B:315:SER:HA	1:B:316:PRO:HD3	1.95	0.43
1:D:76:MET:O	1:D:80:GLN:HG3	2.19	0.43
1:D:265:ILE:CD1	1:D:296:GLN:HG3	2.39	0.43
1:D:94:GLN:HE21	1:D:351:PHE:H	1.65	0.43
1:A:397:VAL:HG23	1:B:105:THR:HG23	2.00	0.42
1:B:190:LYS:HB2	1:B:197:LYS:HG2	2.00	0.42
1:A:130:ARG:HA	1:A:133:GLN:NE2	2.34	0.42
1:B:255:ARG:HG2	1:B:255:ARG:NH1	2.34	0.42
1:B:324:LEU:HD21	4:B:1620:HOH:O	2.18	0.42
1:D:11:GLU:H	1:D:11:GLU:CD	2.22	0.42
1:D:300:ALA:O	1:D:303:ALA:HB3	2.19	0.42
1:A:397:VAL:HG21	1:B:106:TYR:O	2.20	0.42
1:A:370:MET:O	1:A:374:VAL:HG23	2.20	0.42
1:B:200:ILE:HG13	1:B:200:ILE:H	1.63	0.42
1:D:130:ARG:NH1	1:D:133:GLN:HE22	2.15	0.42
1:D:315:SER:HA	1:D:316:PRO:HD3	1.70	0.42
1:C:94:GLN:HE22	1:C:350:GLY:N	2.17	0.42
1:B:269:ILE:O	1:B:273:LYS:HG3	2.19	0.42
1:D:321:LYS:NZ	1:D:326:ASP:OD1	2.53	0.42
1:C:388:TYR:CZ	1:C:390:ALA:HB3	2.54	0.42
1:D:397:VAL:CG2	1:D:397:VAL:O	2.66	0.42
4:C:1749:HOH:O	1:D:374:VAL:HG13	2.20	0.42
1:B:375:GLU:O	1:B:379:ARG:HG3	2.20	0.42
1:D:135:ALA:HA	4:D:1585:HOH:O	2.19	0.42
1:A:246:GLN:N	1:A:247:PRO:CD	2.82	0.41
1:A:276:ALA:HB3	1:A:277:PRO:HD3	2.03	0.41
1:C:321:LYS:HD3	1:D:378:GLU:OE2	2.20	0.41
1:B:88:ILE:CD1	1:B:128:LEU:HD11	2.51	0.41
1:C:59:GLN:HE22	1:C:86:LYS:HB3	1.85	0.41
1:A:243:GLU:HG3	4:A:1213:HOH:O	2.21	0.41
1:B:388:TYR:CZ	1:B:390:ALA:HB3	2.56	0.41
1:A:333:GLN:CA	1:A:344:GLN:HE22	2.33	0.41
1:A:283:TRP:HB2	1:A:311:ALA:HB3	2.03	0.41
1:D:147:LEU:HD23	1:D:147:LEU:HA	1.85	0.41
1:D:266:GLU:HG2	4:D:1780:HOH:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:51:ARG:HG2	4:C:1392:HOH:O	2.20	0.41
1:B:273:LYS:HD3	1:B:304:GLU:OE1	2.20	0.41
1:D:21:PRO:O	1:D:24:LYS:HB2	2.21	0.41
1:B:284:MET:HE3	1:B:286:THR:HG22	2.02	0.41
1:A:93:TRP:CD1	3:A:500:PYR:H33	2.56	0.41
1:C:269:ILE:HG23	1:C:273:LYS:HE3	2.03	0.41
1:D:234:ALA:O	1:D:263:ASN:HB3	2.21	0.41
1:C:397:VAL:HG22	1:D:106:TYR:C	2.41	0.41
1:C:404:ARG:HD3	4:C:1704:HOH:O	2.20	0.41
1:B:152:ALA:O	1:B:179:SER:HA	2.21	0.41
1:A:180:HIS:HB3	1:A:226:ILE:HB	2.03	0.41
1:D:319:ASN:C	1:D:319:ASN:HD22	2.24	0.40
1:B:82:ARG:HD2	4:B:1855:HOH:O	2.21	0.40
1:B:42:VAL:CG2	1:C:147:LEU:HD12	2.48	0.40
1:B:264:GLY:C	1:B:267:PRO:HD2	2.42	0.40
1:C:369:GLN:HB3	1:D:333:GLN:HG3	2.03	0.40
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.85	0.40
1:A:24:LYS:HE3	1:A:25:ASP:CG	2.39	0.40
1:D:53:ALA:HB3	1:D:222:PRO:HG2	2.03	0.40
1:B:130:ARG:HA	1:B:133:GLN:NE2	2.37	0.40
1:A:284:MET:SD	1:A:297:PHE:CD1	3.15	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	425/429 (99%)	415 (98%)	10 (2%)	0	100	100
1	B	425/429 (99%)	415 (98%)	10 (2%)	0	100	100
1	C	425/429 (99%)	417 (98%)	8 (2%)	0	100	100
1	D	425/429 (99%)	413 (97%)	12 (3%)	0	100	100
All	All	1700/1716 (99%)	1660 (98%)	40 (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	337/339 (99%)	327 (97%)	10 (3%)	53	34
1	B	337/339 (99%)	329 (98%)	8 (2%)	61	44
1	C	337/339 (99%)	330 (98%)	7 (2%)	66	51
1	D	337/339 (99%)	327 (97%)	10 (3%)	53	34
All	All	1348/1356 (99%)	1313 (97%)	35 (3%)	59	41

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	11	GLU
1	A	72	LEU
1	A	90	LEU
1	A	144	GLU
1	A	176	VAL
1	A	191	CYS
1	A	292	GLU
1	A	319	ASN
1	A	391	THR
1	B	72	LEU
1	B	90	LEU
1	B	101	LEU
1	B	144	GLU
1	B	176	VAL
1	B	191	CYS
1	B	200	ILE
1	B	319	ASN
1	C	72	LEU
1	C	90	LEU
1	C	101	LEU
1	C	144	GLU
1	C	191	CYS

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Mol	Chain	Res	Type
1	C	253	ARG
1	C	319	ASN
1	D	24	LYS
1	D	72	LEU
1	D	90	LEU
1	D	142	SER
1	D	144	GLU
1	D	176	VAL
1	D	191	CYS
1	D	283	TRP
1	D	292	GLU
1	D	319	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	75	ASN
1	A	94	GLN
1	A	100	ASN
1	A	104	HIS
1	A	133	GLN
1	A	145	ASN
1	A	163	ASN
1	A	205	HIS
1	A	308	GLN
1	A	319	ASN
1	A	344	GLN
1	A	377	GLN
1	B	12	GLN
1	B	75	ASN
1	B	94	GLN
1	B	100	ASN
1	B	104	HIS
1	B	119	GLN
1	B	133	GLN
1	B	145	ASN
1	B	163	ASN
1	B	180	HIS
1	B	205	HIS
1	B	296	GLN
1	B	319	ASN

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Mol	Chain	Res	Type
1	B	344	GLN
1	B	367	GLN
1	B	377	GLN
1	C	12	GLN
1	C	59	GLN
1	C	75	ASN
1	C	94	GLN
1	C	100	ASN
1	C	104	HIS
1	C	133	GLN
1	C	145	ASN
1	C	163	ASN
1	C	180	HIS
1	C	205	HIS
1	C	319	ASN
1	C	344	GLN
1	C	367	GLN
1	C	377	GLN
1	D	61	HIS
1	D	75	ASN
1	D	94	GLN
1	D	100	ASN
1	D	133	GLN
1	D	145	ASN
1	D	163	ASN
1	D	180	HIS
1	D	319	ASN
1	D	344	GLN
1	D	367	GLN
1	D	377	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	PYR	A	500	1	5,5,5	1.29	1 (20%)	6,6,6	2.35	3 (50%)
3	PYR	B	500	1	5,5,5	1.36	1 (20%)	6,6,6	1.37	0
3	PYR	C	500	1	5,5,5	1.49	1 (20%)	6,6,6	1.16	0
3	PYR	D	500	1	5,5,5	1.41	1 (20%)	6,6,6	1.77	2 (33%)

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
3	PYR	A	500	1	-	0/4/4/4	0/0/0/0
3	PYR	B	500	1	-	0/4/4/4	0/0/0/0
3	PYR	C	500	1	-	0/4/4/4	0/0/0/0
3	PYR	D	500	1	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	500	PYR	C2-C1	-2.73	1.47	1.53
3	D	500	PYR	C2-C1	-2.68	1.47	1.53
3	B	500	PYR	C2-C1	-2.39	1.48	1.53
3	A	500	PYR	C2-C1	-2.36	1.48	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	PYR	O2-C1-C2	3.70	122.53	114.37
3	A	500	PYR	O1-C1-C2	-3.21	111.48	120.73
3	D	500	PYR	O3-C2-C1	2.74	123.71	118.75
3	A	500	PYR	O3-C2-C1	2.10	122.56	118.75
3	D	500	PYR	O2-C1-C2	2.06	118.90	114.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.