

Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 11:20 PM EST

PDB ID	:	1O5Q
Title	:	Crystal Structure of Pyruvate and Mg2+ bound 2-methylisocitrate lyase
		(PrpB) from Salmonella typhimurium
Authors	:	Simanshu, D.K.; Murthy, M.R.N.
Deposited on	:	2003-10-04
Resolution	:	2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive $(\#Entries)$	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		
R _{free}	130704	5042 (2.30-2.30)		
Clashscore	141614	5643 (2.30-2.30)		
Ramachandran outliers	138981	5575 (2.30-2.30)		
Sidechain outliers	138945	5575 (2.30-2.30)		
RSRZ outliers	127900	4938 (2.30-2.30)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain					
1	А	305	% • 71%	16%	·	11%		
1	В	305	71%	15%	•	12%		
1	С	305	5% 62%	26%	•	10%		
1	D	305	3% 59%	27%	·	12%		



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8773 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	971	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	271	2056	1297	356	395	8	0	0	
1	Р	268	Total	С	Ν	0	S	0	0	0
	I D		2030	1280	352	390	8	0	0	0
1	C	275	Total	С	Ν	0	S	0	0	0
	275	2081	1312	360	401	8	0	0	0	
1 D	268	Total	С	Ν	0	S	0	0	0	
		2025	1277	352	388	8		0	U	

• Molecule 1 is a protein called Probable methylisocitrate lyase.

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	MET	-	cloning artifact	UNP Q56062
А	0	ALA	-	cloning artifact	UNP Q56062
А	1	SER	-	cloning artifact	UNP Q56062
А	296	LEU	-	expression tag	UNP Q56062
А	297	GLU	-	expression tag	UNP Q56062
А	298	HIS	-	expression tag	UNP Q56062
А	299	HIS	-	expression tag	UNP Q56062
А	300	HIS	-	expression tag	UNP Q56062
А	301	HIS	-	expression tag	UNP Q56062
А	302	HIS	-	expression tag	UNP Q56062
А	303	HIS	-	expression tag	UNP Q56062
В	-1	MET	-	cloning artifact	UNP Q56062
В	0	ALA	-	cloning artifact	UNP Q56062
В	1	SER	-	cloning artifact	UNP Q56062
В	296	LEU	-	expression tag	UNP Q56062
В	297	GLU	-	expression tag	UNP Q56062
В	298	HIS	-	expression tag	UNP Q56062
В	299	HIS	-	expression tag	UNP Q56062
В	300	HIS	-	expression tag	UNP Q56062
В	301	HIS	-	expression tag	UNP Q56062
В	302	HIS	-	expression tag	UNP Q56062



Chain	Residue	Modelled	Actual	Comment	Reference
В	303	HIS	-	expression tag	UNP Q56062
С	-1	MET	-	cloning artifact	UNP Q56062
С	0	ALA	-	cloning artifact	UNP Q56062
С	1	SER	-	cloning artifact	UNP Q56062
С	296	LEU	-	expression tag	UNP Q56062
С	297	GLU	-	expression tag	UNP Q56062
С	298	HIS	-	expression tag	UNP Q56062
С	299	HIS	-	expression tag	UNP Q56062
С	300	HIS	-	expression tag	UNP Q56062
С	301	HIS	-	expression tag	UNP Q56062
С	302	HIS	-	expression tag	UNP Q56062
С	303	HIS	-	expression tag	UNP Q56062
D	-1	MET	-	cloning artifact	UNP Q56062
D	0	ALA	-	cloning artifact	UNP Q56062
D	1	SER	-	cloning artifact	UNP Q56062
D	296	LEU	-	expression tag	UNP Q56062
D	297	GLU	-	expression tag	UNP Q56062
D	298	HIS	-	expression tag	UNP Q56062
D	299	HIS	-	expression tag	UNP Q56062
D	300	HIS	-	expression tag	UNP Q56062
D	301	HIS	-	expression tag	UNP Q56062
D	302	HIS	-	expression tag	UNP Q56062
D	303	HIS	-	expression tag	UNP Q56062

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Mg 1 1	0	0
2	В	1	Total Mg 1 1	0	0
2	С	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

• Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	167	Total O 167 167	0	0
4	В	182	Total O 182 182	0	0
4	С	113	Total O 113 113	0	0
4	D	91	Total O 91 91	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: Probable methylisocitrate lyase

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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	62.95Å 99.68Å 202.40Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{Posolution} \left(\overset{\circ}{\mathbf{A}} \right)$	19.90 - 2.30	Depositor
Resolution (A)	55.87 - 2.30	EDS
% Data completeness	91.4 (19.90-2.30)	Depositor
(in resolution range)	91.5(55.87-2.30)	EDS
R_{merge}	0.06	Depositor
R _{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	$3.32 (at 2.29 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
B B.	0.200 , 0.251	Depositor
II, II, <i>free</i>	0.190 , 0.240	DCC
R_{free} test set	2653 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	33.8	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , 50.8	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8773	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: 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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.31	0/2086	0.56	0/2832	
1	В	0.34	0/2060	0.58	0/2798	
1	С	0.30	0/2111	0.53	0/2866	
1	D	0.29	0/2055	0.53	0/2791	
All	All	0.31	0/8312	0.55	0/11287	

There are no bond length outliers.

There are no bond angle outliers.

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	А	2056	0	2062	49	0
1	В	2030	0	2032	46	0
1	С	2081	0	2083	90	0
1	D	2025	0	2027	84	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	6	0	0	1	0
3	С	6	0	0	0	0
3	D	6	0	0	0	0
4	А	167	0	0	3	0
4	В	182	0	0	8	0
4	С	113	0	0	7	0
4	D	91	0	0	1	0
All	All	8773	0	8204	244	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 (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:260:GLN:H	1:A:260:GLN:HE21	0.97	0.93
1:C:250:VAL:HG22	1:C:263:VAL:HG11	1.50	0.91
1:B:260:GLN:HE21	1:B:260:GLN:N	1.69	0.90
1:D:260:GLN:HE21	1:D:260:GLN:N	1.71	0.88
1:B:260:GLN:HE21	1:B:260:GLN:H	0.90	0.87
1:D:260:GLN:HE21	1:D:260:GLN:H	0.87	0.87
1:D:260:GLN:H	1:D:260:GLN:NE2	1.72	0.85
1:C:243:MET:HG3	1:D:243:MET:HB2	1.58	0.85
1:C:93:SER:HB3	1:C:96:ASN:ND2	1.92	0.84
1:D:249:LYS:HE3	1:D:249:LYS:HA	1.60	0.83
1:C:260:GLN:H	1:C:260:GLN:HE21	1.27	0.82
1:A:132:VAL:HB	1:A:136:GLU:HG2	1.63	0.81
1:C:14:LEU:HD21	1:C:232:MET:HG2	1.62	0.80
1:C:192:GLU:N	1:C:195:MET:HE3	1.99	0.78
1:C:192:GLU:H	1:C:195:MET:HE3	1.49	0.78
1:B:260:GLN:H	1:B:260:GLN:NE2	1.76	0.76
1:D:114:ILE:HD13	1:D:114:ILE:H	1.50	0.76
1:A:260:GLN:HE21	1:A:260:GLN:N	1.80	0.74
1:D:252:THR:O	1:D:256:GLN:HG3	1.89	0.72
1:C:250:VAL:HG22	1:C:263:VAL:CG1	2.19	0.72
1:A:260:GLN:H	1:A:260:GLN:NE2	1.82	0.71
1:C:57:PRO:HB2	1:C:59:LEU:HD13	1.72	0.70
1:D:91:GLY:HA3	1:D:96:ASN:HB3	1.73	0.70
1:D:249:LYS:HE2	1:D:253:VAL:HG23	1.73	0.69
1:D:190:ILE:HD12	1:D:196:TYR:CE1	2.28	0.69
1:B:5:SER:OG	1:B:8:GLN:HG3	1.93	0.69



	A i a	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:187:PRO:HB2	1:D:190:ILE:HD11	1.75	0.68	
1:A:112:LEU:C	1:A:112:LEU:HD12	2.16	0.66	
1:B:259:THR:OG1	1:B:261:LYS:HG3	1.97	0.64	
1:A:193:LEU:HD12	1:A:193:LEU:H	1.62	0.63	
1:D:132:VAL:CG1	1:D:136:GLU:HB3	2.28	0.63	
1:B:91:GLY:HA3	1:B:96:ASN:CB	2.29	0.62	
1:C:260:GLN:H	1:C:260:GLN:NE2	1.97	0.62	
1:D:132:VAL:HG12	1:D:133:SER:N	2.14	0.62	
1:D:134:LYS:O	1:D:138:VAL:HG23	2.00	0.62	
1:D:197:ARG:HG2	1:D:229:HIS:CD2	2.35	0.62	
1:C:223:ASP:HA	1:C:226:ARG:NH1	2.15	0.61	
1:C:93:SER:H	1:C:96:ASN:HD22	1.47	0.61	
1:A:99:ARG:HG2	1:A:99:ARG:HH11	1.66	0.61	
1:D:223:ASP:HA	1:D:226:ARG:NH1	2.15	0.61	
1:C:269:THR:OG1	1:C:272:GLU:HG3	2.01	0.61	
1:C:191:THR:H	1:C:195:MET:HE3	1.66	0.61	
1:C:223:ASP:HA	1:C:226:ARG:HH12	1.65	0.60	
1:D:111:ALA:CB	1:D:154:VAL:HB	2.32	0.60	
1:C:245:ARG:HD3	4:C:3330:HOH:O	2.02	0.59	
1:C:30:HIS:NE2	1:C:243:MET:CE	2.65	0.59	
1:B:188:GLU:HG2	4:B:2354:HOH:O	2.02	0.59	
1:A:30:HIS:HE1	1:B:244:ASN:ND2	2.00	0.59	
1:A:30:HIS:HE1	1:B:244:ASN:HD22	1.51	0.59	
1:C:14:LEU:HD21	1:C:232:MET:CG	2.31	0.59	
1:A:259:THR:OG1	1:A:261:LYS:HG3	2.02	0.58	
1:D:223:ASP:HA	1:D:226:ARG:HH12	1.68	0.58	
1:C:138:VAL:O	1:C:142:ARG:HG3	2.03	0.58	
1:A:27:ASN:C	1:A:27:ASN:HD22	2.07	0.58	
1:D:111:ALA:HB2	1:D:154:VAL:HB	1.84	0.58	
1:C:208:LEU:HD23	1:C:208:LEU:C	2.24	0.57	
1:C:112:LEU:C	1:C:112:LEU:HD12	2.25	0.57	
1:C:254:LEU:HD11	1:D:235:TYR:CE2	2.39	0.57	
1:A:245:ARG:HD3	4:B:2355:HOH:O	2.04	0.57	
1:A:244:ASN:ND2	1:B:30:HIS:HE1	2.04	0.56	
1:B:99:ARG:HD3	4:B:2441:HOH:O	2.06	0.56	
1:B:112:LEU:HD12	1:B:112:LEU:C	2.26	0.56	
1:B:133:SER:OG	1:B:136:GLU:HG3	2.06	0.55	
1:D:6:PRO:HB2	1:D:110:ALA:HB2	1.88	0.55	
1:D:187:PRO:HB2	1:D:190:ILE:CD1	2.37	0.55	
1:D:112:LEU:HD12	1:D:112:LEU:C	2.27	0.55	
1:A:57:PRO:HA	1:B:277:ILE:HD12	1.88	0.55	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:193:LEU:HD12	1:A:193:LEU:N	2.21	0.55	
1:B:106:LYS:HE2	1:C:107:ALA:O	2.05	0.55	
4:A:1412:HOH:O	1:B:245:ARG:HD3	2.05	0.55	
1:D:187:PRO:CB	1:D:190:ILE:HD11	2.37	0.55	
1:C:5:SER:HB3	1:C:8:GLN:HG3	1.88	0.55	
4:C:3309:HOH:O	1:D:241:ARG:HG2	2.07	0.55	
1:C:116:ASP:O	1:C:132:VAL:HG22	2.07	0.54	
1:C:30:HIS:NE2	1:C:243:MET:HE2	2.22	0.54	
1:A:193:LEU:H	1:A:193:LEU:CD1	2.20	0.54	
1:A:197:ARG:HD3	1:A:228:ALA:HA	1.88	0.54	
1:A:29:ASN:HB2	1:B:51:ALA:O	2.07	0.54	
1:C:257:GLU:O	1:C:259:THR:HG22	2.08	0.54	
1:A:208:LEU:C	1:A:208:LEU:HD23	2.28	0.54	
1:C:192:GLU:HG3	4:C:3415:HOH:O	2.08	0.54	
1:C:30:HIS:HE1	1:D:244:ASN:HD22	1.56	0.54	
1:D:132:VAL:HG12	1:D:136:GLU:HB3	1.90	0.54	
1:C:145:VAL:HG13	1:C:148:ARG:NH2	2.23	0.53	
1:D:14:LEU:HD21	1:D:232:MET:SD	2.48	0.53	
1:C:111:ALA:HB2	1:C:154:VAL:HB	1.91	0.53	
1:A:115:GLU:HA	1:A:158:ARG:O	2.09	0.53	
1:C:134:LYS:O	1:C:138:VAL:HG23	2.08	0.53	
1:A:203:ALA:O	1:A:204:GLN:HB2	2.09	0.53	
1:C:58:ASP:C	1:C:59:LEU:HD12	2.30	0.52	
1:D:161:ALA:CB	1:D:173:ARG:HD2	2.39	0.52	
1:C:30:HIS:HE1	1:D:244:ASN:ND2	2.06	0.52	
1:A:221:THR:OG1	1:A:224:GLU:HG3	2.09	0.52	
1:A:193:LEU:HD11	1:A:220:PHE:CE2	2.45	0.52	
1:B:91:GLY:HA3	1:B:96:ASN:HB3	1.92	0.52	
1:A:113:HIS:HA	1:A:156:MET:O	2.10	0.52	
1:C:30:HIS:HD2	4:C:3349:HOH:O	1.92	0.52	
1:D:259:THR:OG1	1:D:261:LYS:HG3	2.11	0.51	
1:C:111:ALA:CB	1:C:154:VAL:HB	2.40	0.51	
1:B:99:ARG:NH2	1:D:56:LEU:HD11	2.26	0.51	
1:D:137:MET:O	1:D:141:ILE:HG13	2.11	0.51	
1:A:113:HIS:HB3	1:A:156:MET:HB3	1.93	0.51	
1:C:30:HIS:CD2	1:C:243:MET:HE3	2.46	0.51	
1:D:89:GLY:C	1:D:91:GLY:H	2.14	0.51	
1:D:263:VAL:O	1:D:266:ILE:HG12	2.10	0.51	
1:A:14:LEU:HD22	1:A:20:LEU:CD2	2.41	0.50	
1:B:269:THR:OG1	1:B:272:GLU:HG3	2.11	0.50	
1:D:132:VAL:HG11	1:D:136:GLU:HB3	1.93	0.50	



	A + O	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:30:HIS:HD2	4:A:1389:HOH:O	1.93	0.50	
1:B:208:LEU:C	1:B:208:LEU:HD23	2.32	0.50	
1:C:30:HIS:NE2	1:C:243:MET:HE3	2.26	0.50	
1:C:252:THR:CG2	1:C:256:GLN:HE21	2.24	0.50	
1:B:111:ALA:CB	1:B:154:VAL:HB	2.41	0.50	
1:C:141:ILE:O	1:C:145:VAL:HG23	2.11	0.50	
1:D:138:VAL:O	1:D:142:ARG:HG3	2.12	0.50	
1:C:235:TYR:CE2	1:D:254:LEU:HD11	2.47	0.50	
1:C:261:LYS:HD2	4:C:3360:HOH:O	2.12	0.49	
1:B:99:ARG:NH1	4:B:2484:HOH:O	2.44	0.49	
1:D:197:ARG:HG2	1:D:229:HIS:HD2	1.74	0.49	
1:D:240:PHE:O	1:D:243:MET:HG2	2.13	0.49	
1:B:134:LYS:HE2	1:B:172:ASP:OD2	2.13	0.49	
1:C:254:LEU:HD21	1:D:235:TYR:CG	2.47	0.49	
1:C:244:ASN:HD22	1:D:30:HIS:HE1	1.61	0.49	
1:D:145:VAL:HG13	1:D:148:ARG:NH2	2.27	0.49	
1:D:186:PHE:CD2	1:D:186:PHE:C	2.86	0.49	
1:C:5:SER:HB3	1:C:8:GLN:CG	2.43	0.49	
1:A:27:ASN:ND2	1:A:30:HIS:H	2.10	0.49	
1:D:208:LEU:C	1:D:208:LEU:HD23	2.33	0.48	
1:D:20:LEU:HD11	1:D:40:GLN:HB2	1.95	0.48	
1:B:211:ILE:HG22	1:B:211:ILE:O	2.14	0.48	
1:A:226:ARG:HA	4:A:1469:HOH:O	2.13	0.48	
1:C:243:MET:CG	1:D:243:MET:HB2	2.38	0.48	
1:C:186:PHE:C	1:C:186:PHE:CD2	2.87	0.48	
1:D:184:MET:HG2	1:D:206:PRO:HB2	1.94	0.48	
1:B:193:LEU:HB3	1:B:228:ALA:HB2	1.96	0.48	
1:C:213:GLU:CD	1:C:213:GLU:H	2.17	0.48	
1:A:135:GLU:CD	1:A:135:GLU:H	2.18	0.48	
1:C:132:VAL:HB	1:C:136:GLU:HG2	1.95	0.48	
1:C:203:ALA:O	1:C:204:GLN:HB2	2.13	0.47	
1:B:116:ASP:O	1:B:132:VAL:HG22	2.14	0.47	
1:D:114:ILE:HD13	1:D:156:MET:O	2.15	0.47	
1:B:158:ARG:NH1	3:B:2302:PYR:O3	2.47	0.47	
1:B:158:ARG:NH2	1:B:188:GLU:OE2	2.46	0.47	
1:C:254:LEU:HD13	1:C:260:GLN:HB3	1.97	0.47	
1:A:171:LEU:HD22	1:A:202:VAL:HG21	1.97	0.46	
1:A:161:ALA:HB2	1:A:173:ARG:HD2	1.97	0.46	
1:D:214:PHE:HE2	1:D:241:ARG:HD3	1.80	0.46	
1:D:228:ALA:O	1:D:229:HIS:HB2	2.14	0.46	
1:D:87:ASP:O	1:D:114:ILE:HA	2.15	0.46	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:107:ALA:O	1:C:106:LYS:HE2	2.15	0.46	
1:C:35:GLN:HA	1:C:80:LEU:HD11	1.98	0.46	
1:B:36:ARG:HG3	4:B:2430:HOH:O	2.15	0.46	
1:C:193:LEU:HD13	1:C:220:PHE:CE2	2.51	0.46	
1:A:21:GLN:NE2	1:B:254:LEU:HD22	2.31	0.45	
1:A:132:VAL:HB	1:A:136:GLU:CG	2.39	0.45	
1:C:84:VAL:O	1:C:112:LEU:HA	2.16	0.45	
1:B:18:ASN:HA	1:B:19:PRO:HA	1.86	0.45	
1:C:225:LEU:HB3	1:C:230:VAL:HB	1.98	0.45	
1:C:244:ASN:ND2	1:D:30:HIS:HE1	2.14	0.45	
1:D:160:ASP:O	1:D:164:VAL:HG23	2.17	0.45	
1:C:57:PRO:HA	1:D:277:ILE:HD12	1.98	0.45	
1:D:186:PHE:C	1:D:186:PHE:HD2	2.20	0.45	
1:A:111:ALA:HB2	1:A:154:VAL:HB	1.98	0.45	
1:C:280:TYR:O	1:C:284:GLU:HG3	2.16	0.45	
1:A:134:LYS:O	1:A:138:VAL:HG23	2.17	0.45	
1:D:132:VAL:CG1	1:D:133:SER:N	2.78	0.45	
1:A:235:TYR:CG	1:B:254:LEU:HD11	2.52	0.45	
1:C:138:VAL:HG13	1:C:180:ALA:HB2	1.97	0.45	
1:A:101:VAL:HG21	1:A:144:ALA:HA	1.98	0.45	
1:A:106:LYS:HE2	1:D:107:ALA:O	2.17	0.44	
1:C:235:TYR:CG	1:D:254:LEU:HD21	2.52	0.44	
1:D:84:VAL:O	1:D:112:LEU:HA	2.18	0.44	
1:C:186:PHE:C	1:C:186:PHE:HD2	2.20	0.44	
1:D:115:GLU:HA	1:D:158:ARG:O	2.17	0.44	
1:D:158:ARG:HH21	1:D:188:GLU:CD	2.21	0.44	
1:A:132:VAL:CB	1:A:136:GLU:HG2	2.42	0.44	
1:C:190:ILE:HG23	1:C:195:MET:HB2	1.99	0.44	
1:C:213:GLU:HG2	1:C:241:ARG:NE	2.33	0.44	
1:D:135:GLU:O	1:D:138:VAL:HB	2.17	0.44	
1:A:10:PHE:O	1:A:14:LEU:HD23	2.17	0.44	
1:B:278:ASN:ND2	4:B:2469:HOH:O	2.51	0.44	
1:C:26:ILE:HG21	1:C:243:MET:CE	2.48	0.44	
1:C:213:GLU:HG2	1:C:241:ARG:HE	1.82	0.44	
1:D:113:HIS:HB3	1:D:156:MET:HB3	1.99	0.44	
1:A:115:GLU:HG3	1:A:117:GLN:HB2	2.00	0.43	
1:A:14:LEU:HD22	1:A:20:LEU:HD22	2.00	0.43	
1:C:134:LYS:HD3	1:C:176:ALA:HB2	2.00	0.43	
1:D:162:LEU:HD13	1:D:162:LEU:C	2.39	0.43	
1:A:137:MET:HG2	1:A:177:TYR:CZ	2.53	0.43	
1:C:192:GLU:HB2	1:C:195:MET:HE2	2.00	0.43	



	A la C	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:191:THR:N	1:C:195:MET:HE3	2.31	0.43	
1:D:132:VAL:HG12	1:D:133:SER:H	1.83	0.43	
1:D:158:ARG:HA	1:D:186:PHE:HB3	2.00	0.43	
1:B:30:HIS:HD2	4:B:2317:HOH:O	2.01	0.43	
1:C:157:ALA:O	1:C:185:LEU:HD13	2.18	0.43	
1:B:158:ARG:HA	1:B:186:PHE:HB3	2.01	0.43	
1:C:5:SER:HB3	1:C:8:GLN:OE1	2.19	0.43	
1:C:131:ILE:HD13	1:C:161:ALA:HA	2.00	0.43	
1:C:243:MET:HE1	1:D:243:MET:HE1	2.01	0.43	
1:B:43:TYR:CG	1:B:234:LEU:HD11	2.54	0.42	
1:C:277:ILE:HD12	1:D:57:PRO:HA	2.01	0.42	
1:C:91:GLY:HA3	1:C:96:ASN:CB	2.49	0.42	
1:C:173:ARG:HB3	1:C:177:TYR:CZ	2.54	0.42	
1:C:187:PRO:HB2	1:C:190:ILE:CD1	2.49	0.42	
1:D:191:THR:HG22	1:D:216:ALA:O	2.19	0.42	
1:B:263:VAL:O	1:B:267:MET:HG3	2.20	0.42	
1:C:263:VAL:HG13	1:C:266:ILE:HD11	2.00	0.42	
1:B:6:PRO:HB2	1:B:110:ALA:HB2	2.01	0.42	
1:C:263:VAL:HG12	1:C:263:VAL:O	2.20	0.42	
1:D:132:VAL:HG11	1:D:136:GLU:CD	2.39	0.42	
1:D:269:THR:OG1	1:D:272:GLU:HG3	2.19	0.42	
1:C:19:PRO:HD3	1:C:226:ARG:HB2	2.02	0.42	
1:C:98:ALA:O	1:C:102:LYS:HE2	2.20	0.42	
1:B:111:ALA:HB1	1:B:154:VAL:HB	2.02	0.42	
1:B:111:ALA:HB2	1:B:154:VAL:HB	2.02	0.42	
1:C:113:HIS:HA	1:C:156:MET:O	2.20	0.42	
4:C:3361:HOH:O	1:D:245:ARG:HD3	2.19	0.42	
1:D:249:LYS:HE3	1:D:249:LYS:CA	2.42	0.42	
1:D:270:ARG:NH2	4:D:4350:HOH:O	2.52	0.42	
1:D:135:GLU:CD	1:D:135:GLU:H	2.23	0.42	
1:A:158:ARG:HA	1:A:186:PHE:HB3	2.01	0.41	
1:C:72:ARG:HD2	4:C:3331:HOH:O	2.20	0.41	
1:D:114:ILE:HD13	1:D:114:ILE:N	2.26	0.41	
1:D:173:ARG:HB3	1:D:177:TYR:CZ	2.56	0.41	
1:D:234:LEU:HG	1:D:236:PRO:HD3	2.02	0.41	
1:D:217:THR:HA	1:D:218:PRO:HD3	1.92	0.41	
1:B:115:GLU:HB3	1:B:158:ARG:HB3	2.01	0.41	
1:B:217:THR:HB	4:B:2359:HOH:O	2.19	0.41	
1:C:186:PHE:CE2	1:C:210:ASN:HB2	2.56	0.41	
1:A:111:ALA:CB	1:A:154:VAL:HB	2.49	0.41	
1:C:198:ARG:O	1:C:202:VAL:HG23	2.20	0.41	



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:D:43:TYR:CG	1:D:234:LEU:HD11	2.56	0.41
1:D:58:ASP:O	1:D:59:LEU:HD12	2.19	0.41
1:D:97:VAL:HG21	1:D:140:ARG:HG3	2.02	0.41
1:C:134:LYS:HD3	1:C:176:ALA:CB	2.51	0.41
1:C:192:GLU:HB2	1:C:195:MET:HG3	2.03	0.41
1:C:59:LEU:HD11	1:D:279:TYR:CE1	2.56	0.41
1:B:113:HIS:HA	1:B:156:MET:O	2.20	0.41
1:A:112:LEU:C	1:A:112:LEU:CD1	2.87	0.40
1:B:113:HIS:HB3	1:B:156:MET:HB3	2.03	0.40
1:C:115:GLU:OE2	1:C:117:GLN:NE2	2.55	0.40
1:A:68:LEU:O	1:A:72:ARG:HG3	2.20	0.40
1:C:191:THR:H	1:C:195:MET:CE	2.33	0.40
1:A:234:LEU:HG	1:A:236:PRO:HD3	2.04	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	Perce	ntiles
1	А	267/305~(88%)	257~(96%)	8 (3%)	2(1%)	22	26
1	В	264/305~(87%)	258~(98%)	6(2%)	0	100	100
1	С	271/305~(89%)	262 (97%)	9~(3%)	0	100	100
1	D	264/305~(87%)	255~(97%)	7 (3%)	2(1%)	19	23
All	All	1066/1220~(87%)	1032 (97%)	30 (3%)	4 (0%)	34	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	92	SER
1	А	164	VAL



 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
1	D	90	PHE
1	D	92	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	210/239 (88%)	204 (97%)	6 (3%)	42 58
1	В	207/239 (87%)	198 (96%)	9 (4%)	29 40
1	С	212/239 (89%)	206~(97%)	6 (3%)	43 60
1	D	206/239 (86%)	199~(97%)	7(3%)	37 51
All	All	835/956 (87%)	807~(97%)	28 (3%)	37 51

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	27	ASN
1	А	30	HIS
1	А	186	PHE
1	А	245	ARG
1	А	260	GLN
1	А	273	LEU
1	В	14	LEU
1	В	30	HIS
1	В	167	LEU
1	В	186	PHE
1	В	198	ARG
1	В	243	MET
1	В	245	ARG
1	В	254	LEU
1	В	260	GLN
1	С	30	HIS
1	С	185	LEU
1	С	186	PHE
1	С	193	LEU



Conti	Commuted from previous page								
Mol	Chain	Res	Type						
1	С	260	GLN						
1	С	273	LEU						
1	D	30	HIS						
1	D	114	ILE						
1	D	140	ARG						
1	D	186	PHE						
1	D	245	ARG						
1	D	249	LYS						
1	D	260	GLN						

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	8	GLN
1	А	27	ASN
1	А	30	HIS
1	А	35	GLN
1	А	244	ASN
1	А	260	GLN
1	А	281	GLN
1	В	30	HIS
1	В	35	GLN
1	В	117	GLN
1	В	204	GLN
1	В	244	ASN
1	В	260	GLN
1	С	30	HIS
1	С	35	GLN
1	С	96	ASN
1	С	117	GLN
1	С	244	ASN
1	С	256	GLN
1	С	260	GLN
1	С	281	GLN
1	D	8	GLN
1	D	30	HIS
1	D	35	GLN
1	D	96	ASN
1	D	117	GLN
1	D	152	ASN
1	D	204	GLN
1	D	229	HIS



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Mol	Chain	Res	Type
1	D	244	ASN
1	D	260	GLN
1	D	271	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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).

Mal	Turne	Chain	Chain	Chain	Chain	Chain	Chain	Chain	hain Dea Li		Dec	Tink	В	Bond lengths			Bond angles		
INIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2									
3	PYR	D	4302	2	$5,\!5,\!5$	1.42	1 (20%)	3,6,6	2.77	2 (66%)									
3	PYR	В	2302	2	$5,\!5,\!5$	1.41	1 (20%)	3,6,6	2.74	2 (66%)									
3	PYR	А	1302	2	$5,\!5,\!5$	1.48	1 (20%)	3,6,6	2.73	2 (66%)									
3	PYR	С	3302	2	$5,\!5,\!5$	1.40	1 (20%)	3,6,6	2.73	2 (66%)									

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	D	4302	2	-	0/4/4/4	-
3	PYR	В	2302	2	-	0/4/4/4	-
3	PYR	А	1302	2	-	0/4/4/4	-
3	PYR	С	3302	2	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
3	А	1302	PYR	CB-CA	2.29	1.54	1.50
3	С	3302	PYR	CB-CA	2.27	1.54	1.50
3	В	2302	PYR	CB-CA	2.22	1.54	1.50
3	D	4302	PYR	CB-CA	2.05	1.54	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	D	4302	PYR	OXT-C-O	-3.82	114.86	123.61
3	В	2302	PYR	OXT-C-O	-3.80	114.91	123.61
3	С	3302	PYR	OXT-C-O	-3.76	115.01	123.61
3	А	1302	PYR	OXT-C-O	-3.75	115.03	123.61
3	С	3302	PYR	OXT-C-CA	2.50	120.82	113.97
3	А	1302	PYR	OXT-C-CA	2.50	120.80	113.97
3	D	4302	PYR	OXT-C-CA	2.47	120.74	113.97
3	В	2302	PYR	OXT-C-CA	2.46	120.70	113.97

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
3	В	2302	PYR	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	< RSRZ >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	271/305~(88%)	-0.10	4 (1%) 73 79	21, 34, 63, 76	0
1	В	268/305~(87%)	-0.16	1 (0%) 92 95	20, 29, 46, 76	0
1	С	275/305~(90%)	0.11	14 (5%) 28 35	26, 44, 69, 85	0
1	D	268/305~(87%)	0.15	9 (3%) 45 52	26, 46, 72, 87	0
All	All	1082/1220~(88%)	0.00	28 (2%) 56 63	20, 38, 67, 87	0

All (28) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	4	HIS	4.1
1	D	91	GLY	3.9
1	С	164	VAL	3.8
1	А	118	VAL	3.6
1	С	170	ALA	3.1
1	С	130	ALA	3.1
1	С	263	VAL	3.0
1	С	166	GLY	3.0
1	D	95	PHE	2.9
1	D	280	TYR	2.8
1	D	194	SER	2.7
1	А	91	GLY	2.7
1	D	118	VAL	2.7
1	С	131	ILE	2.6
1	С	171	LEU	2.6
1	D	130	ALA	2.6
1	D	138	VAL	2.5
1	D	216	ALA	2.5
1	А	95	PHE	2.4
1	А	189	ALA	2.4
1	В	118	VAL	2.3



Mol	Chain	Res	Type	RSRZ	
1	D	89	GLY	2.3	
1	С	92	SER	2.2	
1	С	163	ALA	2.2	
1	С	256	GLN	2.2	
1	С	167	LEU	2.1	
1	С	118	VAL	2.1	
1	С	162	LEU	2.0	

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	А	1301	1/1	0.80	0.13	33,33,33,33	1
3	PYR	D	4302	6/6	0.88	0.18	49,50,52,53	6
3	PYR	А	1302	6/6	0.93	0.16	29,31,34,34	6
2	MG	D	4301	1/1	0.95	0.09	53,53,53,53	1
3	PYR	С	3302	6/6	0.96	0.13	36,39,41,43	6
3	PYR	В	2302	6/6	0.97	0.14	27,31,33,34	6
2	MG	В	2301	1/1	0.97	0.07	32,32,32,32	1
2	MG	С	3301	1/1	0.97	0.08	49,49,49,49	1

6.5 Other polymers (i)

There are no such residues in this entry.

