



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 01:56 PM EDT

PDB ID : 3UDU
Title : Crystal structure of putative 3-isopropylmalate dehydrogenase from *Campylobacter jejuni*
Authors : Tkaczuk, K.L.; Chruszcz, M.; Grimshaw, S.; Onopriyenko, O.; Savchenko, A.; Anderson, W.F.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2011-10-28
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.27
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) : 2.27

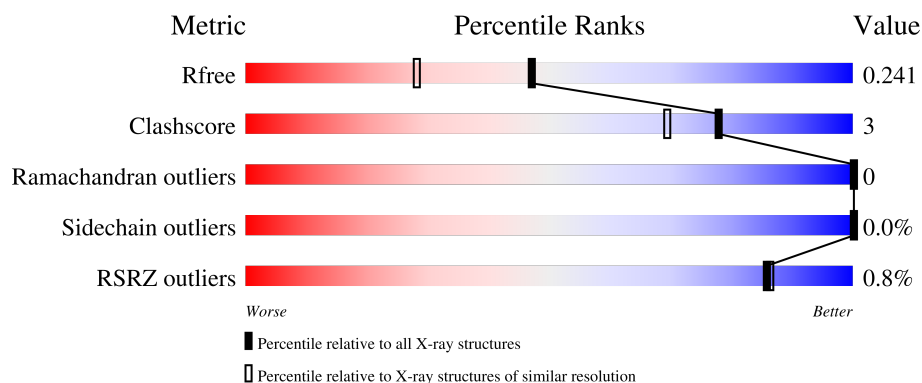
1 Overall quality at a glance

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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (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 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 $\leq 5\%$. 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	361	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	B	361	<div> <div>%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	C	361	<div> <div>2%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	D	361	<div> <div>%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	E	361	<div> <div>%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	361	<div><div></div><div>91%</div><div>8% •</div></div>
1	G	361	<div>%<div><div></div><div>91%</div><div>7% •</div></div></div>
1	H	361	<div>%<div><div></div><div>93%</div><div>5% •</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23703 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 3-isopropylmalate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	1	0
			2758	1757	460	529	12			
1	B	355	Total	C	N	O	S	0	0	0
			2736	1745	452	527	12			
1	C	351	Total	C	N	O	S	0	0	0
			2689	1717	444	516	12			
1	D	356	Total	C	N	O	S	0	0	0
			2741	1748	453	528	12			
1	E	355	Total	C	N	O	S	0	0	0
			2738	1745	454	527	12			
1	F	356	Total	C	N	O	S	0	0	0
			2740	1748	453	527	12			
1	G	356	Total	C	N	O	S	0	0	0
			2743	1748	455	528	12			
1	H	354	Total	C	N	O	S	0	0	0
			2717	1734	451	520	12			

There are 32 discrepancies between the modelled and reference sequences:

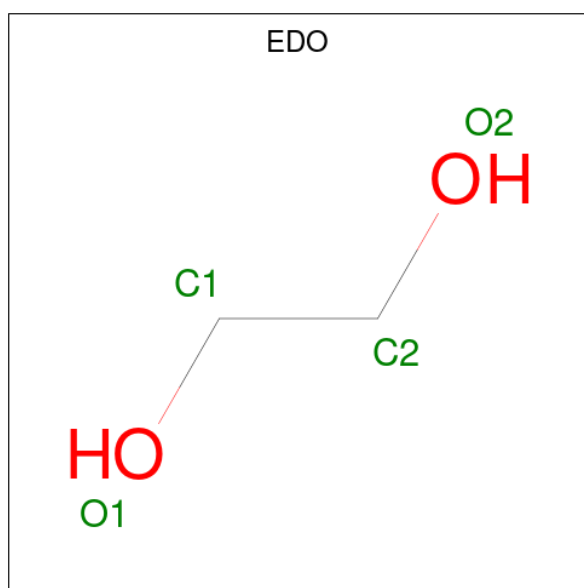
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9PLW0
A	-1	ASN	-	expression tag	UNP Q9PLW0
A	0	ALA	-	expression tag	UNP Q9PLW0
A	39	LEU	PHE	engineered mutation	UNP Q9PLW0
B	-2	SER	-	expression tag	UNP Q9PLW0
B	-1	ASN	-	expression tag	UNP Q9PLW0
B	0	ALA	-	expression tag	UNP Q9PLW0
B	39	LEU	PHE	engineered mutation	UNP Q9PLW0
C	-2	SER	-	expression tag	UNP Q9PLW0
C	-1	ASN	-	expression tag	UNP Q9PLW0
C	0	ALA	-	expression tag	UNP Q9PLW0
C	39	LEU	PHE	engineered mutation	UNP Q9PLW0
D	-2	SER	-	expression tag	UNP Q9PLW0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASN	-	expression tag	UNP Q9PLW0
D	0	ALA	-	expression tag	UNP Q9PLW0
D	39	LEU	PHE	engineered mutation	UNP Q9PLW0
E	-2	SER	-	expression tag	UNP Q9PLW0
E	-1	ASN	-	expression tag	UNP Q9PLW0
E	0	ALA	-	expression tag	UNP Q9PLW0
E	39	LEU	PHE	engineered mutation	UNP Q9PLW0
F	-2	SER	-	expression tag	UNP Q9PLW0
F	-1	ASN	-	expression tag	UNP Q9PLW0
F	0	ALA	-	expression tag	UNP Q9PLW0
F	39	LEU	PHE	engineered mutation	UNP Q9PLW0
G	-2	SER	-	expression tag	UNP Q9PLW0
G	-1	ASN	-	expression tag	UNP Q9PLW0
G	0	ALA	-	expression tag	UNP Q9PLW0
G	39	LEU	PHE	engineered mutation	UNP Q9PLW0
H	-2	SER	-	expression tag	UNP Q9PLW0
H	-1	ASN	-	expression tag	UNP Q9PLW0
H	0	ALA	-	expression tag	UNP Q9PLW0
H	39	LEU	PHE	engineered mutation	UNP Q9PLW0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Cl	0	0
			1	1		

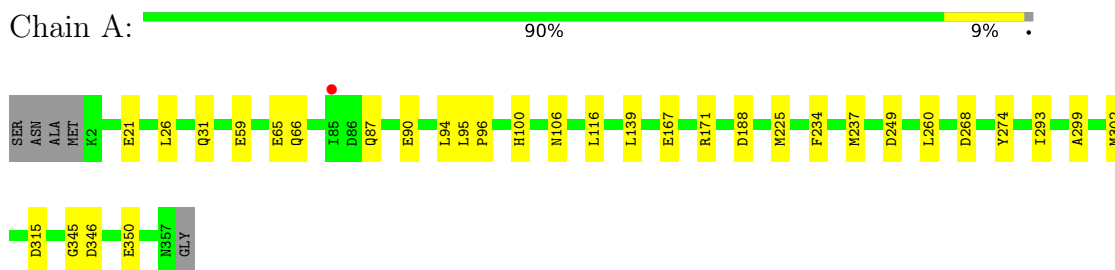
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	256	Total	O	0	0
			256	256		
4	B	242	Total	O	0	0
			242	242		
4	C	199	Total	O	0	0
			199	199		
4	D	214	Total	O	0	0
			214	214		
4	E	207	Total	O	0	0
			207	207		
4	F	234	Total	O	0	0
			234	234		
4	G	240	Total	O	0	0
			240	240		
4	H	224	Total	O	0	0
			224	224		

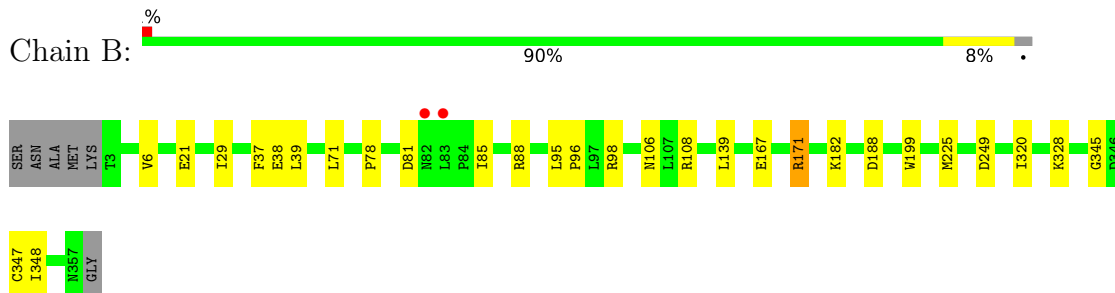
3 Residue-property plots [i](#)

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.

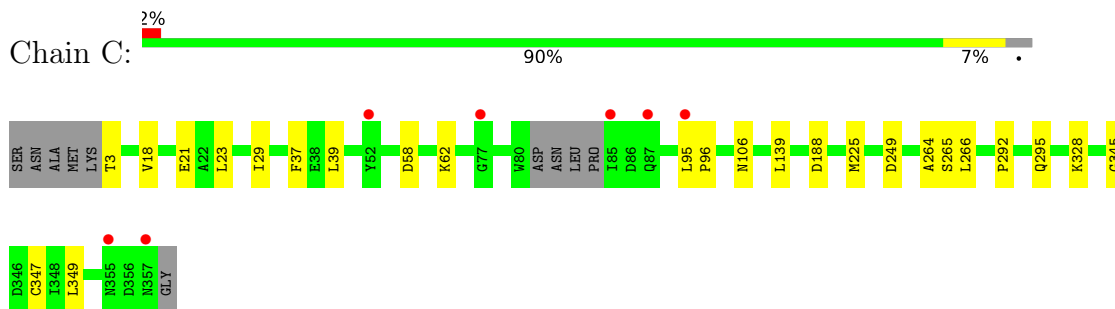
- Molecule 1: 3-isopropylmalate dehydrogenase



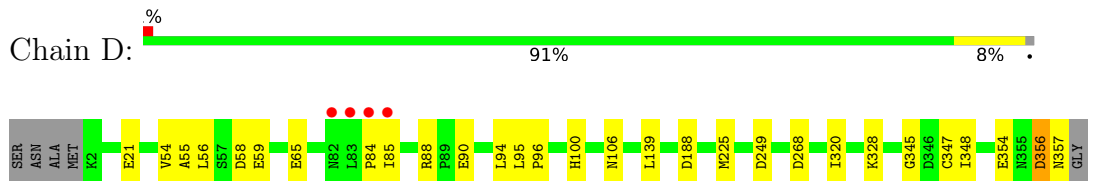
- Molecule 1: 3-isopropylmalate dehydrogenase



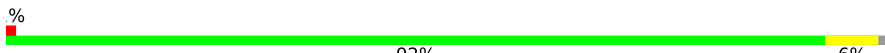
- Molecule 1: 3-isopropylmalate dehydrogenase

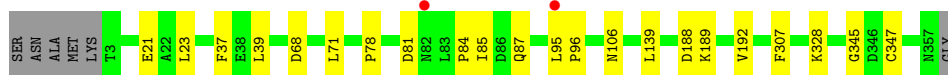


- Molecule 1: 3-isopropylmalate dehydrogenase




● Molecule 1: 3-isopropylmalate dehydrogenase

Chain E:  92% 6% .




● Molecule 1: 3-isopropylmalate dehydrogenase

Chain F:  91% 8% .

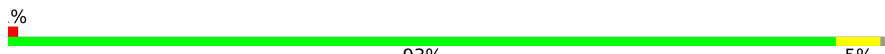


● Molecule 1: 3-isopropylmalate dehydrogenase

Chain G:  91% 7% .



● Molecule 1: 3-isopropylmalate dehydrogenase

Chain H:  93% 5% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.72Å 83.17Å 111.20Å 94.19° 90.07° 89.64°	Depositor
Resolution (Å)	50.00 – 1.85 38.35 – 1.75	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.00-1.85) 93.3 (38.35-1.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.236 0.202 , 0.241	Depositor DCC
R_{free} test set	12780 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.809	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23703	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7000e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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.

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: EDO, CL

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	0.97	1/2801 (0.0%)	0.94	4/3782 (0.1%)
1	B	0.93	1/2779 (0.0%)	0.92	5/3754 (0.1%)
1	C	0.91	0/2730	0.88	2/3686 (0.1%)
1	D	0.93	2/2784 (0.1%)	0.90	3/3761 (0.1%)
1	E	0.95	0/2781	0.90	1/3757 (0.0%)
1	F	0.95	2/2783 (0.1%)	0.94	5/3759 (0.1%)
1	G	0.93	0/2786	0.93	4/3764 (0.1%)
1	H	0.95	0/2759	0.91	1/3726 (0.0%)
All	All	0.94	6/22203 (0.0%)	0.92	25/29989 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	38	GLU	C-N	-5.83	1.20	1.34
1	D	59	GLU	CD-OE1	5.65	1.31	1.25
1	A	59	GLU	CD-OE1	5.45	1.31	1.25
1	B	199	TRP	CD2-CE2	5.45	1.47	1.41
1	F	59	GLU	CD-OE1	5.40	1.31	1.25
1	D	354	GLU	CB-CG	5.22	1.62	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	171	ARG	CG-CD-NE	-5.84	99.54	111.80
1	G	356	ASP	CB-CG-OD1	5.83	123.55	118.30
1	F	356	ASP	CB-CG-OD1	5.82	123.54	118.30
1	F	188	ASP	CB-CG-OD1	5.82	123.53	118.30
1	E	188	ASP	CB-CG-OD1	5.63	123.36	118.30
1	G	356	ASP	CB-CG-OD2	-5.56	113.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	LEU	CB-CG-CD2	-5.56	101.55	111.00
1	C	188	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	98	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	D	356	ASP	CB-CA-C	5.44	121.27	110.40
1	G	94	LEU	CB-CG-CD2	-5.38	101.86	111.00
1	C	349	LEU	CB-CG-CD2	-5.37	101.87	111.00
1	F	356	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	D	188	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	346	ASP	CB-CG-OD1	5.29	123.06	118.30
1	F	346	ASP	CB-CG-OD1	5.29	123.06	118.30
1	H	287	LEU	CB-CG-CD1	5.21	119.86	111.00
1	B	108	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	G	225	MET	CA-CB-CG	5.17	122.08	113.30
1	F	9	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	D	268	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	268	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	315	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	B	188	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2758	0	2797	21	0
1	B	2736	0	2772	20	0
1	C	2689	0	2717	23	0
1	D	2741	0	2774	20	0
1	E	2738	0	2772	13	0
1	F	2740	0	2773	18	0
1	G	2743	0	2774	14	0
1	H	2717	0	2746	12	0
2	A	4	0	6	0	0
2	B	4	0	6	1	0
2	D	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	4	0	6	0	0
2	F	4	0	6	0	0
2	G	4	0	6	0	0
3	C	1	0	0	0	0
4	A	256	0	0	3	0
4	B	242	0	0	1	0
4	C	199	0	0	2	0
4	D	214	0	0	0	0
4	E	207	0	0	0	0
4	F	234	0	0	0	0
4	G	240	0	0	1	0
4	H	224	0	0	3	0
All	All	23703	0	22161	128	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 3.

All (128) 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:18:VAL:HG13	1:C:292:PRO:HA	1.46	0.94
1:E:328:LYS:HD2	1:E:347:CYS:SG	2.19	0.83
1:B:328:LYS:HD2	1:B:347:CYS:SG	2.20	0.82
1:A:350:GLU:HG2	4:A:1705:HOH:O	1.79	0.80
1:C:328:LYS:HD2	1:C:347:CYS:SG	2.24	0.78
1:C:18:VAL:CG1	1:C:292:PRO:HA	2.14	0.77
1:C:58:ASP:O	1:C:62:LYS:HG2	1.86	0.75
1:F:58:ASP:O	1:F:62:LYS:HG3	1.89	0.73
1:D:328:LYS:HD2	1:D:347:CYS:SG	2.29	0.72
1:C:18:VAL:HG13	1:C:292:PRO:CA	2.19	0.72
1:D:320:ILE:CD1	1:D:348:ILE:HD13	2.19	0.72
1:F:328:LYS:HD2	1:F:347:CYS:SG	2.30	0.72
1:E:95:LEU:C	1:E:95:LEU:HD23	2.11	0.71
1:H:328:LYS:HD2	1:H:347:CYS:SG	2.31	0.71
1:C:249:ASP:HB3	1:D:225:MET:HG3	1.74	0.69
1:F:320:ILE:CD1	1:F:348:ILE:HD13	2.22	0.69
1:A:249:ASP:HB3	1:B:225:MET:HG3	1.74	0.69
1:D:84:PRO:HG2	1:F:167:GLU:OE1	1.94	0.66
1:D:84:PRO:CG	1:F:167:GLU:OE1	2.44	0.66
1:B:320:ILE:CD1	1:B:348:ILE:HD13	2.29	0.62
1:D:320:ILE:HD11	1:D:348:ILE:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:208:LYS:NZ	4:H:1810:HOH:O	2.33	0.61
1:C:265:SER:C	1:C:266:LEU:HD12	2.22	0.60
1:A:167:GLU:HG2	1:A:171[A]:ARG:NH2	2.17	0.59
1:F:320:ILE:HD11	1:F:348:ILE:HD13	1.85	0.58
1:F:85:ILE:H	1:F:85:ILE:HD12	1.69	0.58
1:E:23:LEU:HD22	1:E:39:LEU:HD13	1.84	0.58
1:C:266:LEU:HD12	1:C:266:LEU:N	2.18	0.58
1:B:167:GLU:OE2	1:B:171:ARG:NH1	2.37	0.57
1:F:106:ASN:HB2	1:F:139:LEU:HD11	1.87	0.57
1:C:18:VAL:HG11	4:C:1740:HOH:O	2.04	0.55
1:A:66:GLN:NE2	4:A:396:HOH:O	2.39	0.55
1:A:225:MET:HG3	1:B:249:ASP:HB3	1.88	0.55
1:F:320:ILE:CD1	1:F:348:ILE:CD1	2.85	0.55
1:C:266:LEU:N	1:C:266:LEU:CD1	2.70	0.55
1:D:320:ILE:CD1	1:D:348:ILE:CD1	2.85	0.54
1:C:106:ASN:HB2	1:C:139:LEU:HD11	1.89	0.54
1:G:90:GLU:HG3	1:G:94:LEU:HD12	1.90	0.54
1:C:225:MET:HG3	1:D:249:ASP:HB3	1.89	0.53
1:E:95:LEU:HB3	1:E:96:PRO:HD3	1.91	0.52
1:D:356:ASP:O	1:D:357:ASN:C	2.48	0.52
1:D:54:VAL:HG22	1:D:56:LEU:H	1.74	0.52
1:F:189:LYS:HG3	1:F:192:VAL:HG22	1.91	0.52
1:A:87:GLN:NE2	1:G:167:GLU:OE2	2.41	0.51
1:D:106:ASN:HB2	1:D:139:LEU:HD11	1.93	0.51
1:C:264:ALA:HB1	1:C:266:LEU:HD11	1.93	0.50
1:B:85:ILE:HD12	1:B:88:ARG:NH1	2.26	0.50
1:G:188:ASP:O	1:G:219:TYR:HA	2.11	0.50
1:D:84:PRO:HG3	1:F:167:GLU:OE1	2.13	0.49
1:C:249:ASP:HB3	1:D:225:MET:CG	2.42	0.49
1:G:95:LEU:HB3	1:G:96:PRO:HD3	1.94	0.48
1:G:80:TRP:O	1:G:83:LEU:HD13	2.13	0.48
1:G:65:GLU:OE2	1:G:100:HIS:NE2	2.44	0.48
1:C:249:ASP:O	1:D:225:MET:HG2	2.13	0.48
1:H:95:LEU:HB3	1:H:96:PRO:HD3	1.95	0.48
1:B:95:LEU:HB3	1:B:96:PRO:HD3	1.95	0.48
1:F:6:VAL:HB	1:F:39:LEU:HD23	1.97	0.47
1:H:23:LEU:HD22	1:H:39:LEU:HD13	1.97	0.47
1:H:128:GLN:O	1:H:128:GLN:HG3	2.13	0.47
1:A:31:GLN:OE1	4:A:1338:HOH:O	2.20	0.47
1:H:125:GLU:CG	4:H:677:HOH:O	2.62	0.46
1:C:62:LYS:HA	1:C:62:LYS:HD3	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LEU:HD22	1:C:39:LEU:HD13	1.98	0.46
1:B:38:GLU:OE2	2:B:359:EDO:O2	2.30	0.46
1:F:229:LYS:HZ2	1:F:229:LYS:HB3	1.81	0.46
1:A:106:ASN:HB2	1:A:139:LEU:HD11	1.99	0.45
1:B:78:PRO:HA	1:B:81:ASP:OD1	2.17	0.45
1:E:78:PRO:HA	1:E:81:ASP:OD1	2.17	0.45
1:F:65:GLU:OE2	1:F:100:HIS:NE2	2.48	0.45
1:F:85:ILE:HD12	1:F:85:ILE:N	2.31	0.45
1:E:189:LYS:HG3	1:E:192:VAL:HG22	1.99	0.45
1:F:95:LEU:HB3	1:F:96:PRO:HD3	1.98	0.45
1:B:182:LYS:NZ	4:B:802:HOH:O	2.33	0.45
1:G:260:LEU:HD22	1:G:293:ILE:HG21	1.99	0.44
1:D:95:LEU:HB3	1:D:96:PRO:HD3	1.99	0.44
1:A:116:LEU:CD1	1:A:260:LEU:HD11	2.46	0.44
1:C:18:VAL:HG12	1:C:295:GLN:CB	2.47	0.44
1:D:21:GLU:OE1	1:D:345:GLY:HA3	2.18	0.44
1:E:84:PRO:HG2	1:E:87:GLN:NE2	2.33	0.44
1:F:21:GLU:OE1	1:F:345:GLY:HA3	2.18	0.44
1:H:37:PHE:HB3	1:H:39:LEU:HG	2.00	0.44
1:B:320:ILE:CD1	1:B:348:ILE:CD1	2.95	0.43
1:G:85:ILE:HD12	1:G:85:ILE:H	1.83	0.43
1:H:106:ASN:HB2	1:H:139:LEU:HD11	1.99	0.43
1:A:90:GLU:HG3	1:A:94:LEU:HD12	1.99	0.43
1:A:249:ASP:HB3	1:B:225:MET:CG	2.45	0.43
1:D:65:GLU:OE2	1:D:100:HIS:NE2	2.49	0.43
1:E:106:ASN:HB2	1:E:139:LEU:HD11	1.99	0.43
1:A:249:ASP:O	1:B:225:MET:HG2	2.18	0.43
1:C:21:GLU:OE1	1:C:345:GLY:HA3	2.18	0.43
1:A:225:MET:HG2	1:B:249:ASP:O	2.18	0.43
1:E:21:GLU:OE1	1:E:345:GLY:HA3	2.18	0.43
1:A:167:GLU:OE1	1:A:171[A]:ARG:NH2	2.52	0.43
1:G:274:TYR:CZ	1:G:302:MET:HA	2.54	0.43
1:A:21:GLU:OE1	1:A:345:GLY:HA3	2.19	0.42
1:C:37:PHE:HB3	1:C:39:LEU:HG	2.01	0.42
1:F:29:ILE:HD13	1:F:29:ILE:HA	1.95	0.42
1:B:6:VAL:HB	1:B:39:LEU:HD23	2.02	0.42
1:E:85:ILE:H	1:E:85:ILE:HD12	1.85	0.42
1:A:274:TYR:CZ	1:A:302:MET:HA	2.54	0.42
1:H:21:GLU:OE1	1:H:345:GLY:HA3	2.18	0.42
1:G:26:LEU:HD21	1:G:299:ALA:HB1	2.02	0.42
1:C:95:LEU:HB3	1:C:96:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:GLU:OE1	1:G:345:GLY:HA3	2.20	0.42
1:A:260:LEU:HD22	1:A:293:ILE:HG21	2.02	0.42
1:B:29:ILE:HD13	1:B:29:ILE:HA	1.81	0.42
1:A:26:LEU:HD21	1:A:299:ALA:HB1	2.02	0.41
1:B:21:GLU:OE1	1:B:345:GLY:HA3	2.19	0.41
1:B:106:ASN:HB2	1:B:139:LEU:HD11	2.02	0.41
1:E:37:PHE:HB3	1:E:39:LEU:HG	2.03	0.41
1:G:286:HIS:ND1	4:G:1790:HOH:O	2.30	0.41
1:A:95:LEU:HB3	1:A:96:PRO:HD3	2.02	0.41
1:G:148:GLN:NE2	1:G:157:ASP:OD2	2.46	0.41
1:D:85:ILE:HD12	1:D:88:ARG:NH1	2.36	0.41
1:H:274:TYR:CZ	1:H:302:MET:HA	2.56	0.41
1:A:65:GLU:OE2	1:A:100:HIS:NE2	2.52	0.41
1:B:37:PHE:HB3	1:B:39:LEU:HG	2.03	0.41
1:C:3:THR:N	4:C:1823:HOH:O	2.53	0.41
1:D:90:GLU:HG3	1:D:94:LEU:HD12	2.02	0.41
1:H:125:GLU:HG3	4:H:677:HOH:O	2.20	0.41
1:H:328:LYS:CD	1:H:347:CYS:SG	3.07	0.41
1:A:234:PHE:CZ	1:A:237:MET:HE1	2.56	0.41
1:C:29:ILE:HD13	1:C:29:ILE:HA	1.98	0.41
1:E:68:ASP:HB2	1:E:307:PHE:HE1	1.85	0.41
1:D:54:VAL:HG22	1:D:55:ALA:N	2.36	0.40
1:B:85:ILE:HD12	1:B:88:ARG:HH11	1.86	0.40
1:E:71:LEU:HD12	1:E:71:LEU:HA	1.95	0.40
1:G:6:VAL:HB	1:G:39:LEU:HD23	2.03	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	355/361 (98%)	341 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	353/361 (98%)	341 (97%)	12 (3%)	0	100	100
1	C	347/361 (96%)	334 (96%)	13 (4%)	0	100	100
1	D	354/361 (98%)	343 (97%)	11 (3%)	0	100	100
1	E	353/361 (98%)	340 (96%)	13 (4%)	0	100	100
1	F	354/361 (98%)	341 (96%)	13 (4%)	0	100	100
1	G	354/361 (98%)	340 (96%)	14 (4%)	0	100	100
1	H	350/361 (97%)	337 (96%)	13 (4%)	0	100	100
All	All	2820/2888 (98%)	2717 (96%)	103 (4%)	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	295/298 (99%)	295 (100%)	0	100	100
1	B	293/298 (98%)	293 (100%)	0	100	100
1	C	285/298 (96%)	285 (100%)	0	100	100
1	D	293/298 (98%)	292 (100%)	1 (0%)	92	91
1	E	293/298 (98%)	293 (100%)	0	100	100
1	F	293/298 (98%)	293 (100%)	0	100	100
1	G	293/298 (98%)	293 (100%)	0	100	100
1	H	288/298 (97%)	288 (100%)	0	100	100
All	All	2333/2384 (98%)	2332 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	58	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	B	31	GLN
1	B	40	ASN
1	C	357	ASN
1	D	118	HIS
1	E	82	ASN
1	E	87	GLN
1	E	118	HIS
1	H	148	GLN
1	H	357	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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\# Z > 2$
2	EDO	A	359	-	3,3,3	0.64	0	2,2,2	0.60	0
2	EDO	F	359	-	3,3,3	0.53	0	2,2,2	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	G	359	-	3,3,3	0.89	0	2,2,2	0.72	0
2	EDO	D	359	-	3,3,3	0.50	0	2,2,2	0.31	0
2	EDO	E	359	-	3,3,3	0.43	0	2,2,2	0.64	0
2	EDO	B	359	-	3,3,3	0.39	0	2,2,2	0.96	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	EDO	A	359	-	-	1/1/1/1	-
2	EDO	F	359	-	-	0/1/1/1	-
2	EDO	G	359	-	-	1/1/1/1	-
2	EDO	D	359	-	-	1/1/1/1	-
2	EDO	E	359	-	-	1/1/1/1	-
2	EDO	B	359	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	359	EDO	O1-C1-C2-O2
2	D	359	EDO	O1-C1-C2-O2
2	G	359	EDO	O1-C1-C2-O2
2	A	359	EDO	O1-C1-C2-O2
2	E	359	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	359	EDO	1	0

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, 95th 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	A	356/361 (98%)	-0.17	1 (0%) 94 93	17, 26, 41, 63	0
1	B	355/361 (98%)	-0.11	2 (0%) 89 89	17, 26, 44, 63	0
1	C	351/361 (97%)	-0.03	7 (1%) 65 64	17, 29, 52, 72	0
1	D	356/361 (98%)	-0.15	4 (1%) 80 81	18, 27, 46, 71	0
1	E	355/361 (98%)	-0.14	2 (0%) 89 89	16, 27, 44, 62	0
1	F	356/361 (98%)	-0.14	1 (0%) 94 93	16, 26, 45, 64	0
1	G	356/361 (98%)	-0.13	2 (0%) 89 89	17, 26, 43, 61	0
1	H	354/361 (98%)	-0.06	3 (0%) 86 86	17, 28, 52, 81	0
All	All	2839/2888 (98%)	-0.12	22 (0%) 86 86	16, 27, 46, 81	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	ILE	5.3
1	D	84	PRO	3.6
1	F	82	ASN	3.5
1	D	85	ILE	3.5
1	D	83	LEU	3.3
1	C	77	GLY	3.1
1	H	78	PRO	3.0
1	D	82	ASN	2.9
1	G	357	ASN	2.7
1	C	52	TYR	2.5
1	E	95	LEU	2.5
1	H	280	SER	2.5
1	G	85	ILE	2.4
1	C	357	ASN	2.4
1	C	355	ASN	2.3
1	C	95	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	87	GLN	2.2
1	B	82	ASN	2.2
1	B	83	LEU	2.2
1	C	85	ILE	2.1
1	H	258	LEU	2.1
1	E	82	ASN	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, 95th 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	EDO	A	359	4/4	0.88	0.13	29,34,37,41	0
3	CL	C	359	1/1	0.88	0.07	64,64,64,64	0
2	EDO	B	359	4/4	0.89	0.18	40,42,43,48	0
2	EDO	G	359	4/4	0.91	0.11	29,31,32,33	0
2	EDO	D	359	4/4	0.93	0.13	27,33,34,35	0
2	EDO	E	359	4/4	0.96	0.07	24,26,28,32	0
2	EDO	F	359	4/4	0.97	0.10	28,31,34,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.