



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:43 PM UTC

PDB ID : 3R4Q / pdb_00003r4q
Title : Crystal structure of Lactoylglutathione lyase from *Agrobacterium tumefaciens*
Authors : Agarwal, R.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on : 2011-03-17
Resolution : 2.51 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

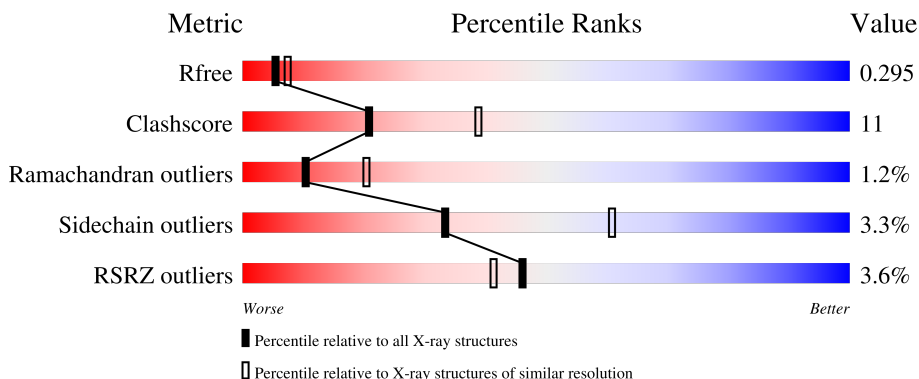
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 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	160	0% 62% 21% • 14%
1	B	160	2% 64% 17% •• 16%
1	C	160	0% 63% 18% • 16%
1	D	160	2% 63% 19% • 16%
1	E	160	8% 52% 28% • 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IPA	A	4572	-	-	-	X
3	IPA	B	4571	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5510 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 Lactoylglutathione lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	0	0
			1088	698	183	202	5			
1	B	134	Total	C	N	O	S	0	0	0
			1068	686	179	198	5			
1	C	134	Total	C	N	O	S	0	0	0
			1068	686	179	198	5			
1	D	134	Total	C	N	O	S	0	0	0
			1062	684	178	195	5			
1	E	133	Total	C	N	O	S	0	0	0
			1058	682	176	195	5			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q7CXA0
A	2	VAL	-	expression tag	UNP Q7CXA0
A	139	ALA	-	expression tag	UNP Q7CXA0
A	140	GLU	-	expression tag	UNP Q7CXA0
A	141	ASN	-	expression tag	UNP Q7CXA0
A	142	LEU	-	expression tag	UNP Q7CXA0
A	143	TYR	-	expression tag	UNP Q7CXA0
A	144	PHE	-	expression tag	UNP Q7CXA0
A	145	GLN	-	expression tag	UNP Q7CXA0
A	146	SER	-	expression tag	UNP Q7CXA0
A	147	HIS	-	expression tag	UNP Q7CXA0
A	148	HIS	-	expression tag	UNP Q7CXA0
A	149	HIS	-	expression tag	UNP Q7CXA0
A	150	HIS	-	expression tag	UNP Q7CXA0
A	151	HIS	-	expression tag	UNP Q7CXA0
A	152	HIS	-	expression tag	UNP Q7CXA0
A	153	TRP	-	expression tag	UNP Q7CXA0
A	154	SER	-	expression tag	UNP Q7CXA0
A	155	HIS	-	expression tag	UNP Q7CXA0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	156	PRO	-	expression tag	UNP Q7CXA0
A	157	GLN	-	expression tag	UNP Q7CXA0
A	158	PHE	-	expression tag	UNP Q7CXA0
A	159	GLU	-	expression tag	UNP Q7CXA0
A	160	LYS	-	expression tag	UNP Q7CXA0
B	1	MET	-	expression tag	UNP Q7CXA0
B	2	VAL	-	expression tag	UNP Q7CXA0
B	139	ALA	-	expression tag	UNP Q7CXA0
B	140	GLU	-	expression tag	UNP Q7CXA0
B	141	ASN	-	expression tag	UNP Q7CXA0
B	142	LEU	-	expression tag	UNP Q7CXA0
B	143	TYR	-	expression tag	UNP Q7CXA0
B	144	PHE	-	expression tag	UNP Q7CXA0
B	145	GLN	-	expression tag	UNP Q7CXA0
B	146	SER	-	expression tag	UNP Q7CXA0
B	147	HIS	-	expression tag	UNP Q7CXA0
B	148	HIS	-	expression tag	UNP Q7CXA0
B	149	HIS	-	expression tag	UNP Q7CXA0
B	150	HIS	-	expression tag	UNP Q7CXA0
B	151	HIS	-	expression tag	UNP Q7CXA0
B	152	HIS	-	expression tag	UNP Q7CXA0
B	153	TRP	-	expression tag	UNP Q7CXA0
B	154	SER	-	expression tag	UNP Q7CXA0
B	155	HIS	-	expression tag	UNP Q7CXA0
B	156	PRO	-	expression tag	UNP Q7CXA0
B	157	GLN	-	expression tag	UNP Q7CXA0
B	158	PHE	-	expression tag	UNP Q7CXA0
B	159	GLU	-	expression tag	UNP Q7CXA0
B	160	LYS	-	expression tag	UNP Q7CXA0
C	1	MET	-	expression tag	UNP Q7CXA0
C	2	VAL	-	expression tag	UNP Q7CXA0
C	139	ALA	-	expression tag	UNP Q7CXA0
C	140	GLU	-	expression tag	UNP Q7CXA0
C	141	ASN	-	expression tag	UNP Q7CXA0
C	142	LEU	-	expression tag	UNP Q7CXA0
C	143	TYR	-	expression tag	UNP Q7CXA0
C	144	PHE	-	expression tag	UNP Q7CXA0
C	145	GLN	-	expression tag	UNP Q7CXA0
C	146	SER	-	expression tag	UNP Q7CXA0
C	147	HIS	-	expression tag	UNP Q7CXA0
C	148	HIS	-	expression tag	UNP Q7CXA0
C	149	HIS	-	expression tag	UNP Q7CXA0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	150	HIS	-	expression tag	UNP Q7CXA0
C	151	HIS	-	expression tag	UNP Q7CXA0
C	152	HIS	-	expression tag	UNP Q7CXA0
C	153	TRP	-	expression tag	UNP Q7CXA0
C	154	SER	-	expression tag	UNP Q7CXA0
C	155	HIS	-	expression tag	UNP Q7CXA0
C	156	PRO	-	expression tag	UNP Q7CXA0
C	157	GLN	-	expression tag	UNP Q7CXA0
C	158	PHE	-	expression tag	UNP Q7CXA0
C	159	GLU	-	expression tag	UNP Q7CXA0
C	160	LYS	-	expression tag	UNP Q7CXA0
D	1	MET	-	expression tag	UNP Q7CXA0
D	2	VAL	-	expression tag	UNP Q7CXA0
D	139	ALA	-	expression tag	UNP Q7CXA0
D	140	GLU	-	expression tag	UNP Q7CXA0
D	141	ASN	-	expression tag	UNP Q7CXA0
D	142	LEU	-	expression tag	UNP Q7CXA0
D	143	TYR	-	expression tag	UNP Q7CXA0
D	144	PHE	-	expression tag	UNP Q7CXA0
D	145	GLN	-	expression tag	UNP Q7CXA0
D	146	SER	-	expression tag	UNP Q7CXA0
D	147	HIS	-	expression tag	UNP Q7CXA0
D	148	HIS	-	expression tag	UNP Q7CXA0
D	149	HIS	-	expression tag	UNP Q7CXA0
D	150	HIS	-	expression tag	UNP Q7CXA0
D	151	HIS	-	expression tag	UNP Q7CXA0
D	152	HIS	-	expression tag	UNP Q7CXA0
D	153	TRP	-	expression tag	UNP Q7CXA0
D	154	SER	-	expression tag	UNP Q7CXA0
D	155	HIS	-	expression tag	UNP Q7CXA0
D	156	PRO	-	expression tag	UNP Q7CXA0
D	157	GLN	-	expression tag	UNP Q7CXA0
D	158	PHE	-	expression tag	UNP Q7CXA0
D	159	GLU	-	expression tag	UNP Q7CXA0
D	160	LYS	-	expression tag	UNP Q7CXA0
E	1	MET	-	expression tag	UNP Q7CXA0
E	2	VAL	-	expression tag	UNP Q7CXA0
E	139	ALA	-	expression tag	UNP Q7CXA0
E	140	GLU	-	expression tag	UNP Q7CXA0
E	141	ASN	-	expression tag	UNP Q7CXA0
E	142	LEU	-	expression tag	UNP Q7CXA0
E	143	TYR	-	expression tag	UNP Q7CXA0

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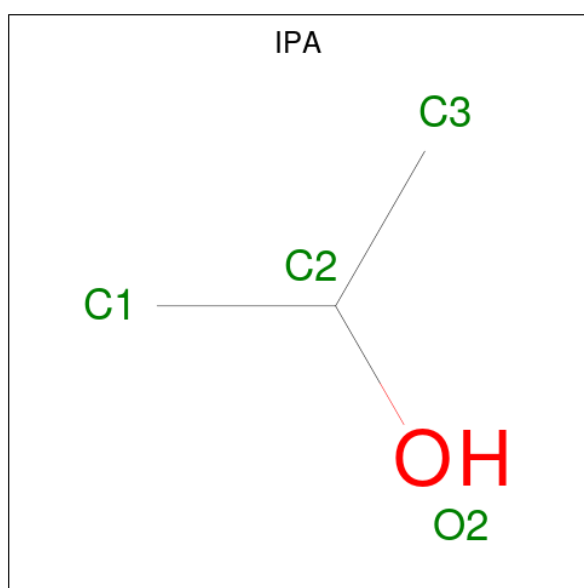
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Chain	Residue	Modelled	Actual	Comment	Reference
E	144	PHE	-	expression tag	UNP Q7CXA0
E	145	GLN	-	expression tag	UNP Q7CXA0
E	146	SER	-	expression tag	UNP Q7CXA0
E	147	HIS	-	expression tag	UNP Q7CXA0
E	148	HIS	-	expression tag	UNP Q7CXA0
E	149	HIS	-	expression tag	UNP Q7CXA0
E	150	HIS	-	expression tag	UNP Q7CXA0
E	151	HIS	-	expression tag	UNP Q7CXA0
E	152	HIS	-	expression tag	UNP Q7CXA0
E	153	TRP	-	expression tag	UNP Q7CXA0
E	154	SER	-	expression tag	UNP Q7CXA0
E	155	HIS	-	expression tag	UNP Q7CXA0
E	156	PRO	-	expression tag	UNP Q7CXA0
E	157	GLN	-	expression tag	UNP Q7CXA0
E	158	PHE	-	expression tag	UNP Q7CXA0
E	159	GLU	-	expression tag	UNP Q7CXA0
E	160	LYS	-	expression tag	UNP Q7CXA0

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Co 1 1	0	0

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		
3	B	1	Total	C	O	0	0
			4	3	1		

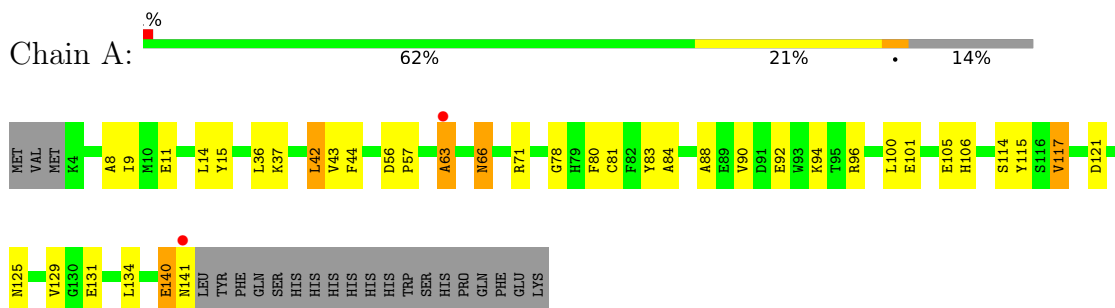
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	32	Total	O	0	0
			32	32		
4	C	36	Total	O	0	0
			36	36		
4	D	42	Total	O	0	0
			42	42		
4	E	9	Total	O	0	0
			9	9		

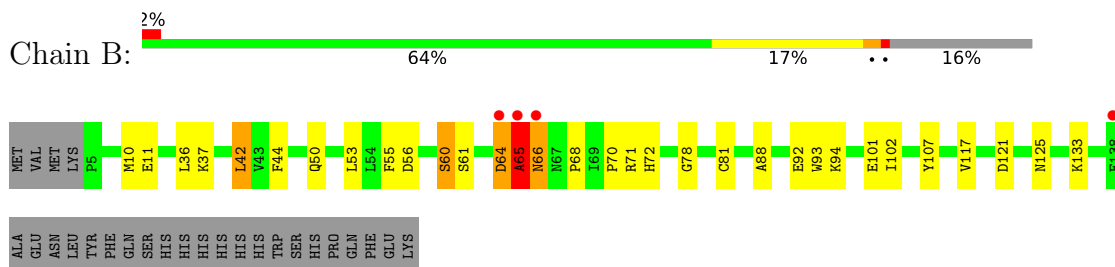
3 Residue-property plots [i](#)

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.

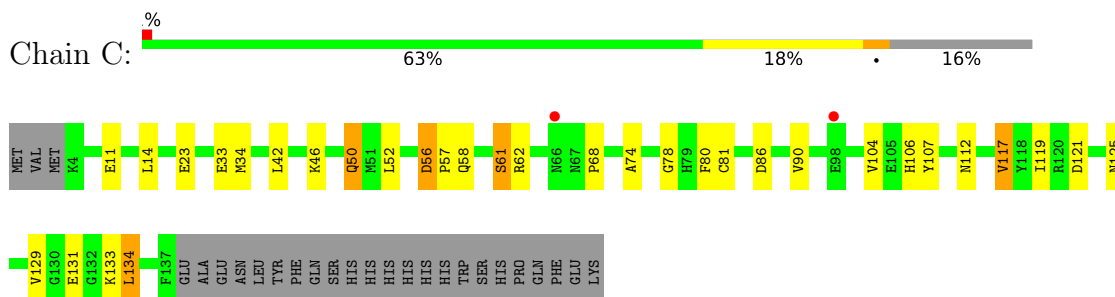
- Molecule 1: Lactoylglutathione lyase



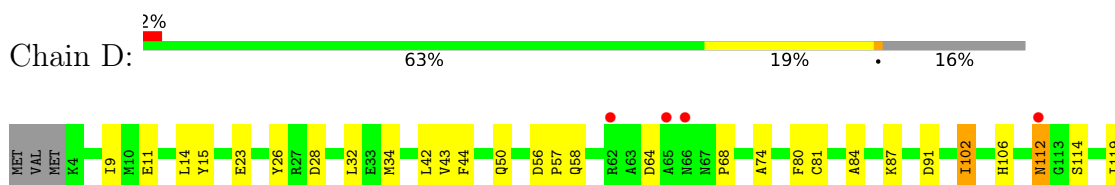
- Molecule 1: Lactoylglutathione lyase

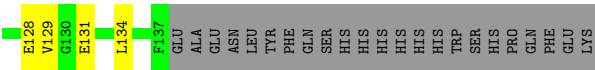


- Molecule 1: Lactoylglutathione lyase

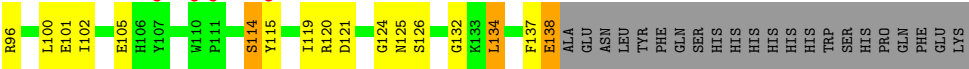
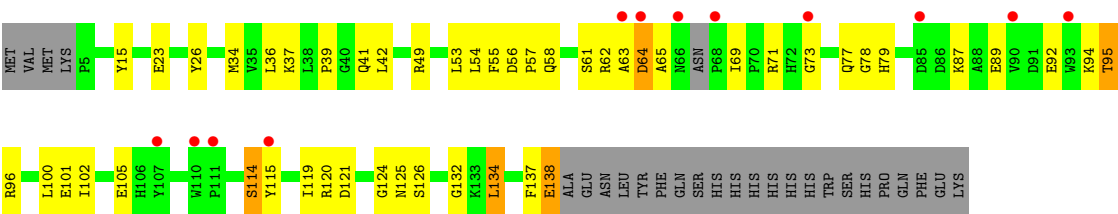


- Molecule 1: Lactoylglutathione lyase





● Molecule 1: Lactoylglutathione lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.53Å 202.52Å 50.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 2.51 49.42 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.42-2.51) 97.6 (49.42-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.60 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.296 0.230 , 0.295	Depositor DCC
R_{free} test set	744 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5510	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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

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	0.51	0/1121	0.94	5/1523 (0.3%)
1	B	0.58	0/1101	1.03	5/1494 (0.3%)
1	C	0.53	0/1101	0.95	4/1495 (0.3%)
1	D	0.62	0/1095	1.03	3/1487 (0.2%)
1	E	0.57	0/1090	1.05	6/1476 (0.4%)
All	All	0.56	0/5508	1.00	23/7475 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	ALA	N-CA-C	-9.86	89.79	110.80
1	E	42	LEU	N-CA-C	7.27	119.92	108.79
1	B	56	ASP	N-CA-C	-6.95	96.03	108.47
1	E	94	LYS	N-CA-C	-6.56	104.05	111.07
1	E	121	ASP	N-CA-C	-6.53	102.62	110.13
1	E	102	ILE	N-CA-C	-6.53	101.17	107.76
1	A	121	ASP	N-CA-C	-6.19	103.01	110.13
1	C	62	ARG	N-CA-C	6.12	118.68	110.35
1	C	56	ASP	N-CA-C	-6.01	97.72	108.47
1	A	56	ASP	N-CA-C	-5.95	96.67	109.81
1	D	56	ASP	N-CA-C	-5.74	97.12	109.81
1	C	42	LEU	N-CA-C	5.67	117.47	108.79
1	C	121	ASP	N-CA-C	-5.64	103.64	110.13
1	A	42	LEU	N-CA-C	5.58	117.33	108.79
1	D	102	ILE	N-CA-C	-5.43	102.27	107.76
1	E	64	ASP	N-CA-C	5.39	122.29	110.80
1	A	115	TYR	N-CA-C	5.35	118.30	109.85
1	B	102	ILE	N-CA-C	-5.27	101.86	107.77
1	E	56	ASP	N-CA-C	-5.27	99.20	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ASP	N-CA-C	-5.22	102.45	110.07
1	B	42	LEU	N-CA-C	5.20	116.42	108.42
1	A	63	ALA	N-CA-C	5.10	117.56	107.98
1	D	64	ASP	N-CA-C	5.09	117.89	109.85

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	1088	0	1011	30	0
1	B	1068	0	1001	22	0
1	C	1068	0	1000	26	0
1	D	1062	0	994	28	0
1	E	1058	0	993	29	0
2	A	1	0	0	0	0
3	A	4	0	8	0	0
3	B	4	0	8	0	0
4	A	38	0	0	0	0
4	B	32	0	0	0	0
4	C	36	0	0	0	0
4	D	42	0	0	1	0
4	E	9	0	0	2	0
All	All	5510	0	5015	115	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 11.

All (115) 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:78:GLY:H	1:C:125:ASN:HD22	1.14	0.96
1:B:78:GLY:H	1:B:125:ASN:HD22	1.13	0.94
1:A:78:GLY:H	1:A:125:ASN:HD22	1.15	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ASN:HD22	1:D:112:ASN:H	1.25	0.82
1:D:114:SER:HB3	1:D:134:LEU:HD12	1.67	0.77
1:C:78:GLY:H	1:C:125:ASN:ND2	1.81	0.76
1:D:112:ASN:HD22	1:D:112:ASN:N	1.84	0.75
1:A:63:ALA:HA	1:A:71:ARG:HD3	1.70	0.74
1:C:50:GLN:HE22	1:D:50:GLN:HE21	1.36	0.73
1:A:78:GLY:H	1:A:125:ASN:ND2	1.88	0.71
1:B:60:SER:HB2	1:B:72:HIS:O	1.90	0.70
1:C:78:GLY:N	1:C:125:ASN:HD22	1.88	0.69
1:A:9:ILE:H	1:B:50:GLN:NE2	1.92	0.68
1:B:78:GLY:H	1:B:125:ASN:ND2	1.89	0.67
1:B:65:ALA:O	1:B:66:ASN:HB2	1.95	0.65
1:A:8:ALA:HB1	1:B:50:GLN:HE22	1.61	0.64
1:C:90:VAL:HG13	1:C:117:VAL:HG22	1.79	0.64
1:A:36:LEU:HD12	1:E:37:LYS:O	1.98	0.64
1:E:114:SER:HB3	1:E:134:LEU:HD12	1.79	0.64
1:E:137:PHE:O	1:E:138:GLU:HB2	1.99	0.63
1:C:50:GLN:HE22	1:D:50:GLN:NE2	1.96	0.63
1:A:81:CYS:HB3	1:B:11:GLU:HB2	1.81	0.62
1:E:15:TYR:HB3	1:E:57:PRO:HD3	1.82	0.62
1:D:15:TYR:HB3	1:D:57:PRO:HD3	1.83	0.61
1:E:89:GLU:O	1:E:92:GLU:HB2	2.00	0.61
1:A:78:GLY:N	1:A:125:ASN:HD22	1.95	0.60
1:A:37:LYS:HD3	1:A:43:VAL:HG22	1.83	0.60
1:A:9:ILE:H	1:B:50:GLN:HE21	1.49	0.59
1:D:112:ASN:H	1:D:112:ASN:ND2	1.99	0.59
1:A:90:VAL:HG13	1:A:117:VAL:HG22	1.85	0.59
1:E:63:ALA:O	1:E:65:ALA:N	2.36	0.59
1:C:14:LEU:HD12	1:C:52:LEU:HD11	1.83	0.59
1:A:100:LEU:O	1:A:101:GLU:HB2	2.03	0.57
1:C:74:ALA:HB1	1:D:74:ALA:HB1	1.85	0.57
1:E:96:ARG:HH11	1:E:96:ARG:HG3	1.69	0.57
1:C:11:GLU:HB2	1:D:81:CYS:HB3	1.86	0.56
1:C:57:PRO:O	1:C:61:SER:HB2	2.05	0.56
1:C:117:VAL:HG23	1:C:129:VAL:HB	1.88	0.56
1:A:42:LEU:HD22	1:A:44:PHE:CZ	2.41	0.55
1:E:92:GLU:O	1:E:95:THR:HB	2.07	0.55
1:C:23:GLU:OE1	1:C:34:MET:HE1	2.07	0.53
1:A:117:VAL:HG23	1:A:129:VAL:HB	1.90	0.53
1:E:78:GLY:H	1:E:125:ASN:HD22	1.55	0.53
1:D:102:ILE:HG22	1:D:119:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HB3	1:B:55:PHE:CE1	2.45	0.52
1:D:26:TYR:HB3	1:D:32:LEU:HD12	1.90	0.52
1:C:50:GLN:NE2	1:D:50:GLN:HE21	2.06	0.52
1:E:134:LEU:HD22	4:E:170:HOH:O	2.11	0.51
1:E:15:TYR:CE1	1:E:73:GLY:HA2	2.45	0.51
1:E:105:GLU:CD	1:E:120:ARG:HE	2.19	0.51
1:B:78:GLY:N	1:B:125:ASN:HD22	1.96	0.50
1:C:56:ASP:OD1	1:C:58:GLN:HG2	2.11	0.50
1:A:106:HIS:CE1	1:B:68:PRO:HB2	2.46	0.50
1:E:23:GLU:HG3	1:E:34:MET:HE1	1.94	0.50
1:C:131:GLU:O	1:C:134:LEU:HB2	2.12	0.50
1:A:88:ALA:O	1:A:92:GLU:HG3	2.12	0.50
1:A:94:LYS:HB2	1:A:117:VAL:HG11	1.94	0.49
1:E:62:ARG:O	1:E:63:ALA:C	2.56	0.49
1:E:96:ARG:CZ	1:E:100:LEU:HD11	2.44	0.48
1:C:50:GLN:HG3	1:D:9:ILE:HG12	1.93	0.48
1:D:84:ALA:O	1:D:131:GLU:HA	2.13	0.48
1:A:114:SER:HB2	1:A:134:LEU:HD12	1.95	0.48
1:C:68:PRO:HB2	1:D:106:HIS:CE1	2.48	0.48
1:A:36:LEU:HD13	1:E:39:PRO:HD2	1.96	0.48
1:B:61:SER:O	1:B:71:ARG:HD2	2.13	0.47
1:B:36:LEU:HD23	1:B:37:LYS:N	2.29	0.47
1:E:79:HIS:HB2	1:E:126:SER:HB3	1.97	0.47
1:E:61:SER:O	1:E:71:ARG:HD2	2.14	0.47
1:E:132:GLY:O	1:E:137:PHE:HB2	2.15	0.47
1:E:26:TYR:CD2	1:E:54:LEU:HD11	2.50	0.46
1:E:78:GLY:H	1:E:125:ASN:ND2	2.14	0.46
1:A:14:LEU:HD11	1:A:80:PHE:CD2	2.50	0.45
1:C:14:LEU:HD11	1:C:80:PHE:CE1	2.50	0.45
1:D:14:LEU:HD11	1:D:80:PHE:CE2	2.52	0.45
1:E:15:TYR:CD1	1:E:55:PHE:HB2	2.52	0.45
1:D:112:ASN:N	1:D:112:ASN:ND2	2.57	0.45
1:A:15:TYR:HB3	1:A:57:PRO:HD3	1.99	0.44
1:A:105:GLU:HG2	1:B:70:PRO:HG3	1.99	0.44
1:E:49:ARG:HG3	1:E:49:ARG:HH11	1.81	0.44
1:B:94:LYS:HB2	1:B:117:VAL:HG11	2.00	0.44
1:C:112:ASN:O	1:C:133:LYS:HE3	2.17	0.44
1:A:66:ASN:H	1:A:66:ASN:HD22	1.66	0.44
1:C:86:ASP:HA	1:C:131:GLU:HG2	2.00	0.44
1:E:96:ARG:HG3	1:E:96:ARG:NH1	2.32	0.44
1:E:36:LEU:HD23	1:E:37:LYS:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ASP:CG	1:B:65:ALA:H	2.25	0.43
1:D:28:ASP:HB2	4:D:190:HOH:O	2.19	0.43
1:D:14:LEU:HD11	1:D:80:PHE:CD2	2.53	0.42
1:D:114:SER:CB	1:D:134:LEU:HD12	2.44	0.42
1:D:9:ILE:O	1:D:50:GLN:HG2	2.18	0.42
1:C:107:TYR:HD1	1:C:117:VAL:HG13	1.84	0.42
1:A:11:GLU:HB2	1:B:81:CYS:HB3	2.00	0.42
1:C:33:GLU:HG2	1:C:46:LYS:HB3	2.00	0.42
1:A:140:GLU:O	1:A:141:ASN:CB	2.67	0.42
1:A:83:TYR:HB2	1:B:10:MET:HB2	2.02	0.42
1:A:84:ALA:O	1:A:131:GLU:HA	2.19	0.42
1:D:128:GLU:HG2	1:D:129:VAL:N	2.35	0.42
1:E:77:GLN:HG2	1:E:124:GLY:C	2.44	0.42
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.85	0.41
1:E:58:GLN:O	1:E:62:ARG:HB2	2.20	0.41
1:B:88:ALA:O	1:B:92:GLU:HG3	2.21	0.41
1:C:81:CYS:HB3	1:D:11:GLU:HG3	2.02	0.41
1:E:87:LYS:HE2	1:E:115:TYR:CD1	2.55	0.41
1:A:63:ALA:HB2	1:A:71:ARG:NH1	2.35	0.41
1:B:65:ALA:O	1:B:66:ASN:CB	2.65	0.41
1:C:106:HIS:NE2	1:D:68:PRO:HB2	2.36	0.41
1:A:66:ASN:HD22	1:A:66:ASN:N	2.18	0.41
1:B:42:LEU:HD13	1:B:44:PHE:CE1	2.56	0.41
1:C:50:GLN:HE21	1:D:9:ILE:HB	1.85	0.41
1:D:87:LYS:HG2	1:D:91:ASP:OD2	2.20	0.41
1:C:104:VAL:HA	1:C:119:ILE:HG22	2.03	0.40
1:D:23:GLU:HG3	1:D:43:VAL:HG11	2.02	0.40
1:E:101:GLU:HG3	4:E:169:HOH:O	2.22	0.40
1:B:107:TYR:HD1	1:B:117:VAL:HG12	1.85	0.40
1:D:42:LEU:HD13	1:D:44:PHE:CE1	2.57	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	136/160 (85%)	131 (96%)	4 (3%)	1 (1%)	18	34
1	B	132/160 (82%)	127 (96%)	2 (2%)	3 (2%)	5	8
1	C	132/160 (82%)	127 (96%)	5 (4%)	0	100	100
1	D	132/160 (82%)	126 (96%)	6 (4%)	0	100	100
1	E	129/160 (81%)	111 (86%)	14 (11%)	4 (3%)	3	5
All	All	661/800 (83%)	622 (94%)	31 (5%)	8 (1%)	10	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	ASP
1	B	65	ALA
1	B	66	ASN
1	E	64	ASP
1	E	114	SER
1	A	140	GLU
1	E	119	ILE
1	E	95	THR

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	109/135 (81%)	107 (98%)	2 (2%)	51	77
1	B	109/135 (81%)	105 (96%)	4 (4%)	30	57
1	C	109/135 (81%)	105 (96%)	4 (4%)	30	57
1	D	107/135 (79%)	104 (97%)	3 (3%)	38	66
1	E	107/135 (79%)	102 (95%)	5 (5%)	23	47
All	All	541/675 (80%)	523 (97%)	18 (3%)	33	61

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	117	VAL
1	B	60	SER
1	B	93	TRP
1	B	101	GLU
1	B	133	LYS
1	C	50	GLN
1	C	61	SER
1	C	117	VAL
1	C	134	LEU
1	D	34	MET
1	D	58	GLN
1	D	112	ASN
1	E	41	GLN
1	E	53	LEU
1	E	69	ILE
1	E	134	LEU
1	E	138	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	125	ASN
1	B	50	GLN
1	B	67	ASN
1	B	77	GLN
1	B	125	ASN
1	C	50	GLN
1	C	58	GLN
1	C	106	HIS
1	C	125	ASN
1	D	67	ASN
1	D	112	ASN
1	E	41	GLN
1	E	112	ASN
1	E	125	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	IPA	B	4571	-	3,3,3	0.60	0	3,3,3	0.36	0
3	IPA	A	4572	-	3,3,3	0.64	0	3,3,3	0.34	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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	138/160 (86%)	0.04	2 (1%) 73 70	15, 22, 36, 42	0
1	B	134/160 (83%)	0.03	4 (2%) 52 48	13, 22, 33, 53	0
1	C	134/160 (83%)	-0.03	2 (1%) 72 68	14, 23, 35, 39	0
1	D	134/160 (83%)	0.04	4 (2%) 52 48	15, 22, 39, 54	0
1	E	133/160 (83%)	1.02	12 (9%) 15 13	23, 42, 52, 57	0
All	All	673/800 (84%)	0.22	24 (3%) 46 41	13, 24, 48, 57	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	ASN	4.9
1	B	65	ALA	4.7
1	E	63	ALA	4.0
1	E	66	ASN	3.8
1	D	65	ALA	3.7
1	D	66	ASN	3.4
1	D	112	ASN	3.3
1	B	66	ASN	3.2
1	E	64	ASP	2.9
1	A	63	ALA	2.9
1	E	115	TYR	2.7
1	E	68	PRO	2.7
1	C	66	ASN	2.7
1	E	85	ASP	2.5
1	E	107	TYR	2.5
1	B	64	ASP	2.4
1	E	93	TRP	2.4
1	C	98	GLU	2.3
1	E	111	PRO	2.3
1	E	90	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	62	ARG	2.1
1	B	138	GLU	2.0
1	E	73	GLY	2.0
1	E	110	TRP	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	IPA	A	4572	4/4	0.21	0.67	39,40,40,41	4
3	IPA	B	4571	4/4	0.59	0.51	22,22,22,23	4
2	CO	A	161	1/1	0.86	0.25	49,49,49,49	1

6.5 Other polymers [i](#)

There are no such residues in this entry.