



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 09:49 PM EDT

PDB ID : 6ZNE
Title : MaeB PTA domain R535E mutant
Authors : Lovering, A.L.; Harding, C.J.
Deposited on : 2020-07-06
Resolution : 2.39 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

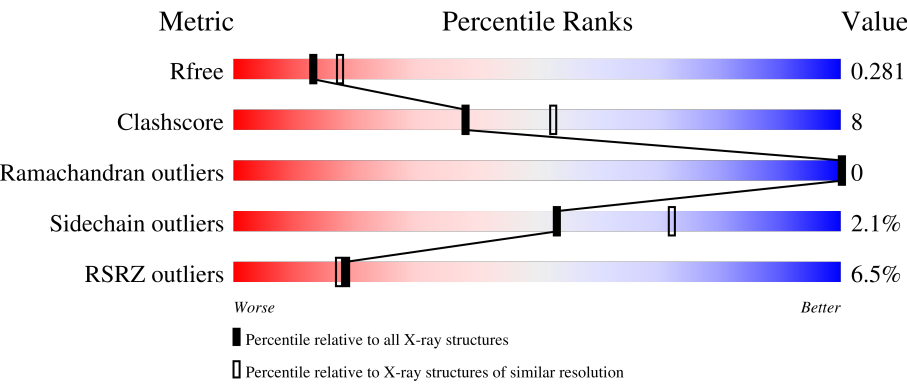
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	362	
1	B	362	
1	C	362	
1	D	362	
1	E	362	

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Mol	Chain	Length	Quality of chain
1	F	362	<div><div></div><div>8%</div><div>79%</div><div>14%</div><div>• 7%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15628 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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2596	1657	441	487	11			
1	B	338	Total	C	N	O	S	0	0	0
			2596	1657	441	487	11			
1	D	338	Total	C	N	O	S	0	0	0
			2596	1657	441	487	11			
1	F	338	Total	C	N	O	S	0	0	0
			2596	1657	441	487	11			
1	E	338	Total	C	N	O	S	0	0	0
			2596	1657	441	487	11			
1	C	339	Total	C	N	O	S	0	0	0
			2601	1660	442	488	11			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	MET	-	initiating methionine	UNP Q6MM15
A	420	GLY	-	expression tag	UNP Q6MM15
A	421	SER	-	expression tag	UNP Q6MM15
A	422	SER	-	expression tag	UNP Q6MM15
A	423	HIS	-	expression tag	UNP Q6MM15
A	424	HIS	-	expression tag	UNP Q6MM15
A	425	HIS	-	expression tag	UNP Q6MM15
A	426	HIS	-	expression tag	UNP Q6MM15
A	427	HIS	-	expression tag	UNP Q6MM15
A	428	HIS	-	expression tag	UNP Q6MM15
A	429	SER	-	expression tag	UNP Q6MM15
A	430	SER	-	expression tag	UNP Q6MM15
A	431	GLY	-	expression tag	UNP Q6MM15
A	432	LEU	-	expression tag	UNP Q6MM15
A	433	VAL	-	expression tag	UNP Q6MM15
A	434	PRO	-	expression tag	UNP Q6MM15
A	435	ALA	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
A	436	GLY	-	expression tag	UNP Q6MM15
A	437	SER	-	expression tag	UNP Q6MM15
A	438	HIS	-	expression tag	UNP Q6MM15
A	535	GLU	ARG	engineered mutation	UNP Q6MM15
B	419	MET	-	initiating methionine	UNP Q6MM15
B	420	GLY	-	expression tag	UNP Q6MM15
B	421	SER	-	expression tag	UNP Q6MM15
B	422	SER	-	expression tag	UNP Q6MM15
B	423	HIS	-	expression tag	UNP Q6MM15
B	424	HIS	-	expression tag	UNP Q6MM15
B	425	HIS	-	expression tag	UNP Q6MM15
B	426	HIS	-	expression tag	UNP Q6MM15
B	427	HIS	-	expression tag	UNP Q6MM15
B	428	HIS	-	expression tag	UNP Q6MM15
B	429	SER	-	expression tag	UNP Q6MM15
B	430	SER	-	expression tag	UNP Q6MM15
B	431	GLY	-	expression tag	UNP Q6MM15
B	432	LEU	-	expression tag	UNP Q6MM15
B	433	VAL	-	expression tag	UNP Q6MM15
B	434	PRO	-	expression tag	UNP Q6MM15
B	435	ALA	-	expression tag	UNP Q6MM15
B	436	GLY	-	expression tag	UNP Q6MM15
B	437	SER	-	expression tag	UNP Q6MM15
B	438	HIS	-	expression tag	UNP Q6MM15
B	535	GLU	ARG	engineered mutation	UNP Q6MM15
D	419	MET	-	initiating methionine	UNP Q6MM15
D	420	GLY	-	expression tag	UNP Q6MM15
D	421	SER	-	expression tag	UNP Q6MM15
D	422	SER	-	expression tag	UNP Q6MM15
D	423	HIS	-	expression tag	UNP Q6MM15
D	424	HIS	-	expression tag	UNP Q6MM15
D	425	HIS	-	expression tag	UNP Q6MM15
D	426	HIS	-	expression tag	UNP Q6MM15
D	427	HIS	-	expression tag	UNP Q6MM15
D	428	HIS	-	expression tag	UNP Q6MM15
D	429	SER	-	expression tag	UNP Q6MM15
D	430	SER	-	expression tag	UNP Q6MM15
D	431	GLY	-	expression tag	UNP Q6MM15
D	432	LEU	-	expression tag	UNP Q6MM15
D	433	VAL	-	expression tag	UNP Q6MM15
D	434	PRO	-	expression tag	UNP Q6MM15
D	435	ALA	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
D	436	GLY	-	expression tag	UNP Q6MM15
D	437	SER	-	expression tag	UNP Q6MM15
D	438	HIS	-	expression tag	UNP Q6MM15
D	535	GLU	ARG	engineered mutation	UNP Q6MM15
F	419	MET	-	initiating methionine	UNP Q6MM15
F	420	GLY	-	expression tag	UNP Q6MM15
F	421	SER	-	expression tag	UNP Q6MM15
F	422	SER	-	expression tag	UNP Q6MM15
F	423	HIS	-	expression tag	UNP Q6MM15
F	424	HIS	-	expression tag	UNP Q6MM15
F	425	HIS	-	expression tag	UNP Q6MM15
F	426	HIS	-	expression tag	UNP Q6MM15
F	427	HIS	-	expression tag	UNP Q6MM15
F	428	HIS	-	expression tag	UNP Q6MM15
F	429	SER	-	expression tag	UNP Q6MM15
F	430	SER	-	expression tag	UNP Q6MM15
F	431	GLY	-	expression tag	UNP Q6MM15
F	432	LEU	-	expression tag	UNP Q6MM15
F	433	VAL	-	expression tag	UNP Q6MM15
F	434	PRO	-	expression tag	UNP Q6MM15
F	435	ALA	-	expression tag	UNP Q6MM15
F	436	GLY	-	expression tag	UNP Q6MM15
F	437	SER	-	expression tag	UNP Q6MM15
F	438	HIS	-	expression tag	UNP Q6MM15
F	535	GLU	ARG	engineered mutation	UNP Q6MM15
E	419	MET	-	initiating methionine	UNP Q6MM15
E	420	GLY	-	expression tag	UNP Q6MM15
E	421	SER	-	expression tag	UNP Q6MM15
E	422	SER	-	expression tag	UNP Q6MM15
E	423	HIS	-	expression tag	UNP Q6MM15
E	424	HIS	-	expression tag	UNP Q6MM15
E	425	HIS	-	expression tag	UNP Q6MM15
E	426	HIS	-	expression tag	UNP Q6MM15
E	427	HIS	-	expression tag	UNP Q6MM15
E	428	HIS	-	expression tag	UNP Q6MM15
E	429	SER	-	expression tag	UNP Q6MM15
E	430	SER	-	expression tag	UNP Q6MM15
E	431	GLY	-	expression tag	UNP Q6MM15
E	432	LEU	-	expression tag	UNP Q6MM15
E	433	VAL	-	expression tag	UNP Q6MM15
E	434	PRO	-	expression tag	UNP Q6MM15
E	435	ALA	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
E	436	GLY	-	expression tag	UNP Q6MM15
E	437	SER	-	expression tag	UNP Q6MM15
E	438	HIS	-	expression tag	UNP Q6MM15
E	535	GLU	ARG	engineered mutation	UNP Q6MM15
C	419	MET	-	initiating methionine	UNP Q6MM15
C	420	GLY	-	expression tag	UNP Q6MM15
C	421	SER	-	expression tag	UNP Q6MM15
C	422	SER	-	expression tag	UNP Q6MM15
C	423	HIS	-	expression tag	UNP Q6MM15
C	424	HIS	-	expression tag	UNP Q6MM15
C	425	HIS	-	expression tag	UNP Q6MM15
C	426	HIS	-	expression tag	UNP Q6MM15
C	427	HIS	-	expression tag	UNP Q6MM15
C	428	HIS	-	expression tag	UNP Q6MM15
C	429	SER	-	expression tag	UNP Q6MM15
C	430	SER	-	expression tag	UNP Q6MM15
C	431	GLY	-	expression tag	UNP Q6MM15
C	432	LEU	-	expression tag	UNP Q6MM15
C	433	VAL	-	expression tag	UNP Q6MM15
C	434	PRO	-	expression tag	UNP Q6MM15
C	435	ALA	-	expression tag	UNP Q6MM15
C	436	GLY	-	expression tag	UNP Q6MM15
C	437	SER	-	expression tag	UNP Q6MM15
C	438	HIS	-	expression tag	UNP Q6MM15
C	535	GLU	ARG	engineered mutation	UNP Q6MM15

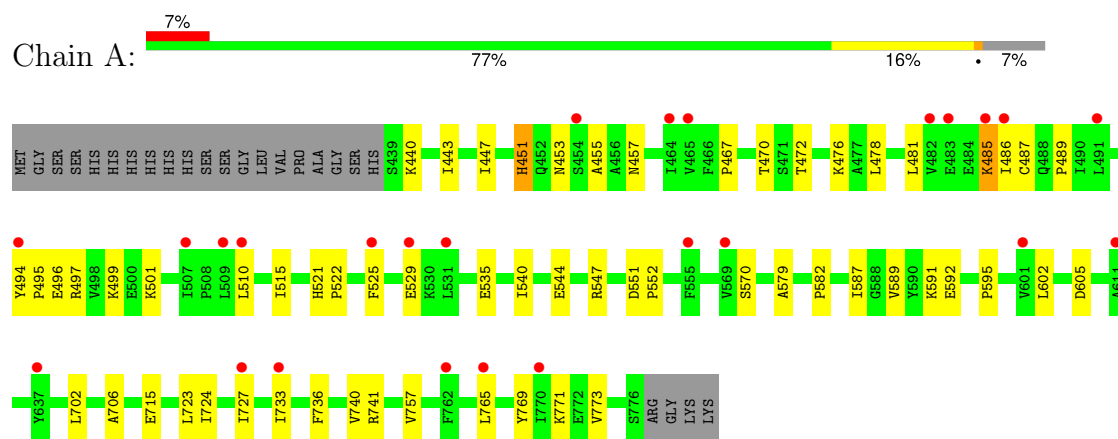
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	9	Total O 9 9	0	0
2	D	10	Total O 10 10	0	0
2	F	2	Total O 2 2	0	0
2	E	9	Total O 9 9	0	0
2	C	7	Total O 7 7	0	0

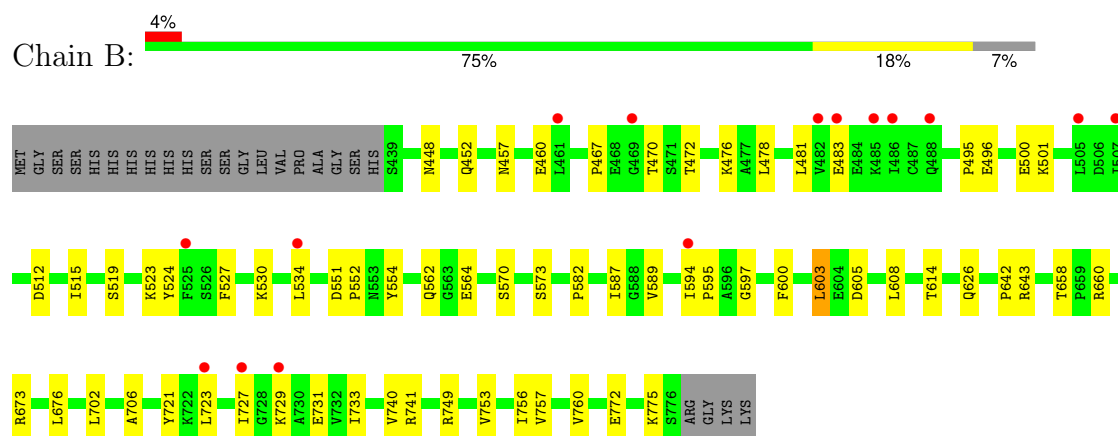
3 Residue-property plots [i](#)

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.

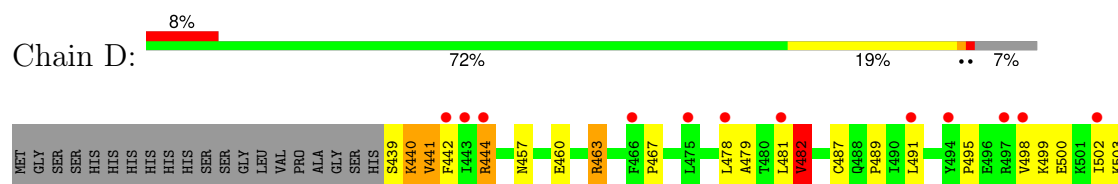
• Molecule 1: Malate dehydrogenase

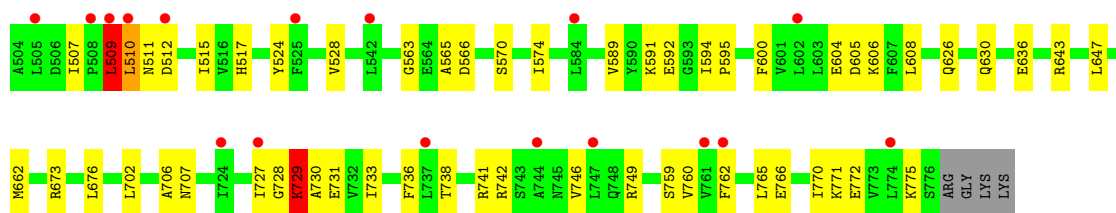


• Molecule 1: Malate dehydrogenase

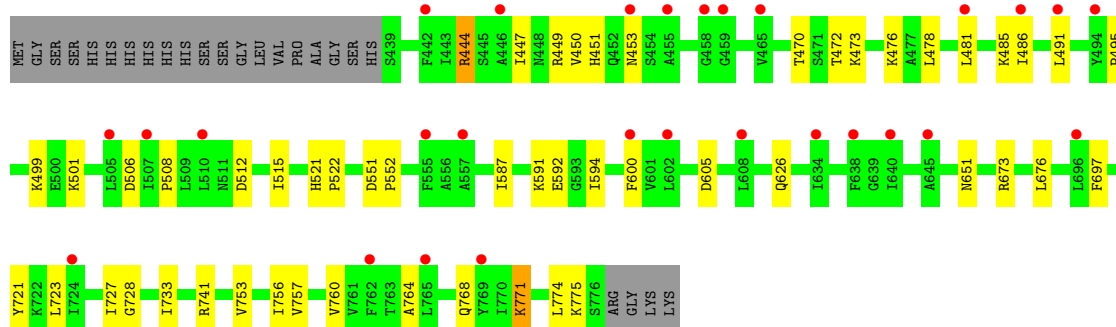
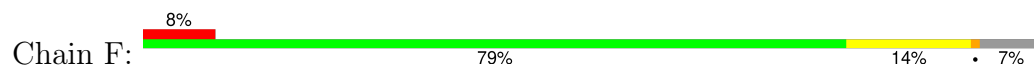


• Molecule 1: Malate dehydrogenase

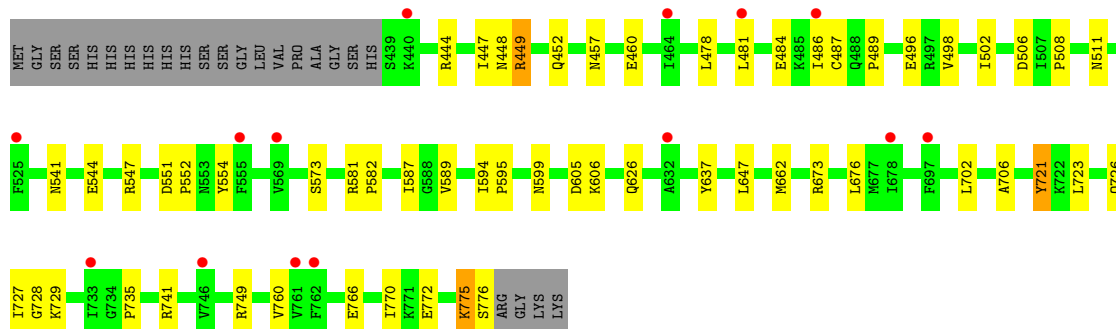
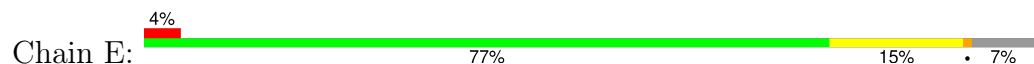




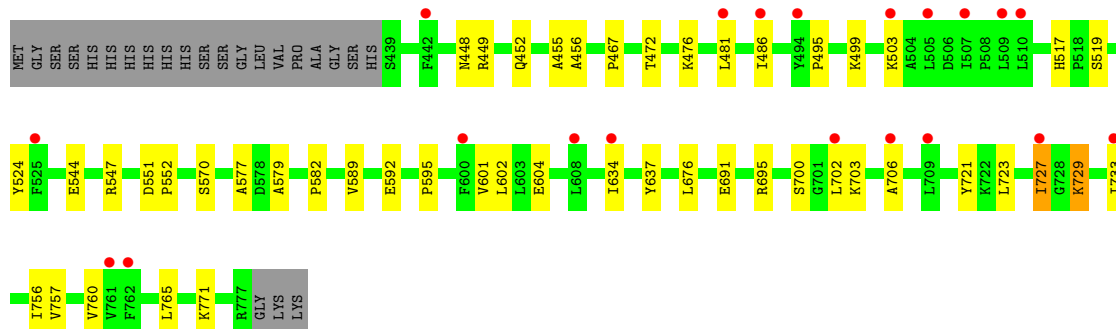
• Molecule 1: Malate dehydrogenase



• Molecule 1: Malate dehydrogenase



• Molecule 1: Malate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.42Å 183.40Å 120.24Å 90.00° 117.03° 90.00°	Depositor
Resolution (Å)	69.66 – 2.39 97.60 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.2 (69.66-2.39) 98.3 (97.60-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.215 , 0.260 0.239 , 0.281	Depositor DCC
R_{free} test set	4767 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15628	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	1/2640 (0.0%)	0.66	1/3574 (0.0%)
1	B	0.53	0/2640	0.66	0/3574
1	C	0.48	0/2645	0.70	3/3581 (0.1%)
1	D	0.49	0/2640	0.78	4/3574 (0.1%)
1	E	0.49	0/2640	0.67	0/3574
1	F	0.47	0/2640	0.64	0/3574
All	All	0.49	1/15845 (0.0%)	0.69	8/21451 (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	D	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	HIS	CG-CD2	-5.66	1.26	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	730	ALA	N-CA-CB	-11.02	94.67	110.10
1	C	455	ALA	N-CA-C	10.72	139.94	111.00
1	D	509	LEU	CA-CB-CG	9.68	137.56	115.30
1	D	729	LYS	N-CA-CB	8.42	125.76	110.60
1	C	456	ALA	N-CA-C	-6.18	94.32	111.00
1	C	456	ALA	CB-CA-C	5.65	118.57	110.10
1	A	510	LEU	CB-CA-C	-5.42	99.89	110.20
1	D	728	GLY	N-CA-C	-5.11	100.31	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	482	VAL	Peptide
1	D	510	LEU	Peptide

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	2596	0	2668	39	0
1	B	2596	0	2668	38	0
1	C	2601	0	2670	38	0
1	D	2596	0	2668	66	0
1	E	2596	0	2668	39	0
1	F	2596	0	2666	40	0
2	A	10	0	0	0	0
2	B	9	0	0	1	0
2	C	7	0	0	1	0
2	D	10	0	0	1	0
2	E	9	0	0	1	0
2	F	2	0	0	0	0
All	All	15628	0	16008	241	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 8.

All (241) 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:D:729:LYS:HE3	1:C:729:LYS:CB	1.31	1.55
1:D:729:LYS:CE	1:C:729:LYS:HB3	1.50	1.41
1:F:453:ASN:OD1	1:F:768:GLN:NE2	1.58	1.31
1:D:729:LYS:CE	1:C:729:LYS:CB	2.14	1.18
1:D:729:LYS:HE3	1:C:729:LYS:HB2	1.22	1.13
1:D:729:LYS:NZ	1:C:729:LYS:HB3	1.69	1.07
1:F:449:ARG:HH12	1:F:453:ASN:HB3	1.21	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:766:GLU:O	1:D:770:ILE:HG13	1.66	0.93
1:E:449:ARG:HG2	1:E:449:ARG:HH11	1.40	0.86
1:D:729:LYS:HE3	1:C:729:LYS:CA	2.06	0.86
1:D:729:LYS:NZ	1:C:729:LYS:O	2.09	0.84
1:D:509:LEU:O	1:D:511:ASN:ND2	2.14	0.81
1:D:591:LYS:HE3	1:D:592:GLU:HG3	1.63	0.81
1:E:676:LEU:O	2:E:801:HOH:O	1.98	0.80
1:A:440:LYS:HA	1:A:443:ILE:HD12	1.67	0.75
1:D:511:ASN:OD1	1:D:512:ASP:N	2.21	0.73
1:C:691:GLU:OE2	1:C:695:ARG:NH2	2.22	0.72
1:D:440:LYS:H	1:D:440:LYS:HD3	1.54	0.71
1:D:482:VAL:HG21	1:D:487:CYS:O	1.90	0.71
1:F:453:ASN:CG	1:F:768:GLN:NE2	2.34	0.71
1:B:589:VAL:HG11	1:B:595:PRO:HD3	1.72	0.71
1:C:589:VAL:HG11	1:C:595:PRO:HD3	1.73	0.70
1:A:496:GLU:HB2	1:A:497:ARG:NH1	2.06	0.70
1:D:499:LYS:O	1:D:502:ILE:HG22	1.91	0.70
1:F:453:ASN:OD1	1:F:768:GLN:CD	2.31	0.69
1:E:444:ARG:NH2	1:E:484:GLU:OE2	2.25	0.69
1:D:511:ASN:CG	1:D:512:ASP:H	1.93	0.69
1:E:496:GLU:OE1	1:E:496:GLU:N	2.26	0.68
1:F:449:ARG:NH1	1:F:453:ASN:HB3	2.04	0.68
1:B:702:LEU:HD21	1:B:706:ALA:HB2	1.76	0.68
1:D:509:LEU:C	1:D:511:ASN:HD22	1.97	0.67
1:B:495:PRO:HA	1:B:515:ILE:HG21	1.76	0.67
1:B:523:LYS:NZ	1:B:564:GLU:OE2	2.29	0.66
1:E:775:LYS:HE2	1:E:776:SER:HB2	1.79	0.64
1:D:729:LYS:HZ1	1:C:729:LYS:C	1.99	0.64
1:A:589:VAL:HG11	1:A:595:PRO:HD3	1.79	0.64
1:C:481:LEU:HD21	1:C:757:VAL:HG13	1.78	0.64
1:C:577:ALA:N	2:C:801:HOH:O	2.08	0.63
1:C:448:ASN:O	1:C:452:GLN:HG3	1.99	0.63
1:A:715:GLU:OE2	1:B:658:THR:HG21	1.98	0.63
1:A:447:ILE:HG23	1:A:486:ILE:HD11	1.81	0.63
1:D:746:VAL:O	2:D:801:HOH:O	2.16	0.63
1:D:589:VAL:HG11	1:D:595:PRO:HD3	1.80	0.62
1:E:726:GLN:O	1:E:729:LYS:NZ	2.33	0.61
1:B:496:GLU:O	1:B:500:GLU:HG2	2.01	0.61
1:A:451:HIS:CD2	1:A:485:LYS:HG2	2.35	0.61
1:A:724:ILE:HD13	1:B:727:ILE:HD11	1.82	0.60
1:D:491:LEU:HB2	1:D:515:ILE:HG12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:ILE:CD1	1:B:727:ILE:HD11	2.31	0.60
1:D:702:LEU:HD21	1:D:706:ALA:HB2	1.84	0.60
1:F:470:THR:O	1:F:501:LYS:NZ	2.30	0.60
1:C:544:GLU:OE1	1:C:547:ARG:NH2	2.31	0.59
1:F:486:ILE:HD11	1:F:760:VAL:HG12	1.85	0.59
1:D:440:LYS:HD3	1:D:440:LYS:N	2.17	0.59
1:E:605:ASP:OD1	1:E:605:ASP:N	2.25	0.58
1:B:723:LEU:O	1:B:727:ILE:HG12	2.03	0.58
1:D:440:LYS:H	1:D:440:LYS:CD	2.09	0.57
1:F:485:LYS:O	1:F:485:LYS:HG2	2.04	0.57
1:E:749:ARG:HG3	1:E:749:ARG:HH11	1.70	0.57
1:D:643:ARG:HB3	1:D:702:LEU:HD11	1.85	0.57
1:A:467:PRO:HG2	1:A:570:SER:HB3	1.88	0.56
1:D:481:LEU:HD13	1:D:760:VAL:HG11	1.87	0.56
1:E:447:ILE:HG23	1:E:486:ILE:HD11	1.87	0.56
1:D:478:LEU:HD23	1:D:481:LEU:HD12	1.87	0.55
1:E:449:ARG:HG2	1:E:449:ARG:NH1	2.18	0.55
1:F:600:PHE:HB2	1:F:733:ILE:HG12	1.87	0.55
1:A:495:PRO:HA	1:A:515:ILE:HG21	1.89	0.55
1:E:448:ASN:O	1:E:452:GLN:HG3	2.05	0.55
1:E:449:ARG:NH1	1:E:637:TYR:OH	2.40	0.55
1:A:481:LEU:HD21	1:A:757:VAL:HG13	1.89	0.55
1:D:509:LEU:HA	1:D:511:ASN:HB3	1.89	0.54
1:E:723:LEU:O	1:E:727:ILE:HG12	2.07	0.54
1:D:509:LEU:O	1:D:509:LEU:HD12	2.07	0.54
1:A:591:LYS:HG2	1:A:592:GLU:N	2.23	0.54
1:A:733:ILE:HG22	1:A:736:PHE:CZ	2.43	0.54
1:F:764:ALA:O	1:F:768:GLN:HG3	2.07	0.53
1:B:448:ASN:O	1:B:452:GLN:HG3	2.08	0.53
1:F:450:VAL:HA	1:F:453:ASN:ND2	2.23	0.53
1:C:723:LEU:O	1:C:727:ILE:HG12	2.09	0.53
1:E:589:VAL:HG11	1:E:595:PRO:HD3	1.90	0.53
1:B:673:ARG:HH11	1:B:676:LEU:HD11	1.74	0.53
1:C:702:LEU:HD11	1:C:706:ALA:HB2	1.91	0.52
1:F:495:PRO:HA	1:F:515:ILE:HG21	1.90	0.52
1:F:673:ARG:HG2	1:F:676:LEU:HD12	1.91	0.52
1:D:511:ASN:CG	1:D:512:ASP:N	2.58	0.52
1:E:647:LEU:O	1:E:662:MET:HG3	2.10	0.52
1:B:600:PHE:HB2	1:B:733:ILE:HG12	1.90	0.52
1:D:594:ILE:HG22	1:D:626:GLN:HG3	1.90	0.52
1:A:496:GLU:OE1	1:A:496:GLU:N	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:487:CYS:O	1:E:489:PRO:HD3	2.11	0.51
1:B:587:ILE:O	1:B:741:ARG:HD3	2.10	0.51
1:A:587:ILE:O	1:A:741:ARG:HD3	2.11	0.51
1:D:741:ARG:HG2	1:D:742:ARG:NH1	2.27	0.50
1:B:600:PHE:HB2	1:B:733:ILE:CG1	2.41	0.50
1:D:479:ALA:HB2	1:D:507:ILE:HG21	1.94	0.50
1:F:485:LYS:O	1:F:485:LYS:CG	2.59	0.50
1:D:478:LEU:HB3	1:D:510:LEU:HD21	1.93	0.50
1:F:600:PHE:HB2	1:F:733:ILE:CG1	2.42	0.50
1:B:501:LYS:NZ	2:B:801:HOH:O	2.42	0.50
1:F:473:LYS:HE2	1:F:753:VAL:HG23	1.93	0.50
1:A:723:LEU:O	1:A:727:ILE:HG12	2.11	0.49
1:B:483:GLU:HA	1:B:483:GLU:OE1	2.11	0.49
1:B:589:VAL:HA	1:B:740:VAL:HA	1.92	0.49
1:F:481:LEU:HD21	1:F:757:VAL:HG13	1.94	0.49
1:D:604:GLU:OE1	1:D:604:GLU:N	2.45	0.49
1:A:605:ASP:OD1	1:A:605:ASP:N	2.34	0.49
1:A:496:GLU:HB2	1:A:497:ARG:HH11	1.76	0.49
1:F:771:LYS:HE2	1:F:775:LYS:HD3	1.95	0.48
1:C:592:GLU:O	1:C:592:GLU:HG3	2.12	0.48
1:D:600:PHE:HB2	1:D:733:ILE:HG12	1.95	0.48
1:B:753:VAL:O	1:B:757:VAL:HG23	2.13	0.48
1:E:573:SER:HA	1:E:749:ARG:NH1	2.28	0.48
1:C:700:SER:O	1:C:703:LYS:NZ	2.28	0.48
1:E:702:LEU:HD21	1:E:706:ALA:HB2	1.96	0.48
1:D:729:LYS:HG2	1:C:729:LYS:HB2	1.95	0.48
1:D:630:GLN:NE2	1:D:738:THR:OG1	2.46	0.48
1:D:463:ARG:HD2	1:D:565:ALA:HA	1.95	0.47
1:A:702:LEU:HD11	1:A:706:ALA:HB2	1.95	0.47
1:B:467:PRO:HG2	1:B:570:SER:HB3	1.96	0.47
1:F:495:PRO:O	1:F:499:LYS:HG3	2.15	0.47
1:D:498:VAL:HG21	1:D:515:ILE:HG21	1.96	0.46
1:D:605:ASP:OD2	1:D:606:LYS:NZ	2.44	0.46
1:A:525:PHE:CE2	1:A:529:GLU:OE2	2.68	0.46
1:F:449:ARG:HD2	1:F:449:ARG:O	2.15	0.46
1:B:573:SER:HA	1:B:749:ARG:NH1	2.31	0.46
1:F:587:ILE:O	1:F:741:ARG:HD3	2.15	0.46
1:D:729:LYS:CG	1:C:729:LYS:HB2	2.46	0.46
1:E:766:GLU:O	1:E:770:ILE:HG13	2.16	0.46
1:B:554:TYR:CE2	1:B:582:PRO:HG3	2.50	0.46
1:D:442:PHE:CE2	1:D:762:PHE:HZ	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:472:THR:CG2	1:F:476:LYS:HE3	2.46	0.46
1:D:500:GLU:HA	1:D:503:LYS:HE3	1.96	0.46
1:F:651:ASN:HB3	1:F:697:PHE:CZ	2.51	0.46
1:B:756:ILE:O	1:B:760:VAL:HG23	2.16	0.45
1:E:544:GLU:OE1	1:E:547:ARG:NH2	2.46	0.45
1:D:441:VAL:HA	1:D:444:ARG:HD2	1.97	0.45
1:F:512:ASP:OD1	1:F:512:ASP:N	2.45	0.45
1:E:749:ARG:HG3	1:E:749:ARG:NH1	2.31	0.45
1:F:723:LEU:O	1:F:727:ILE:HG12	2.15	0.45
1:D:495:PRO:HD3	1:D:517:HIS:HB2	1.97	0.45
1:D:729:LYS:CE	1:C:729:LYS:HB2	2.10	0.45
1:F:551:ASP:HA	1:F:552:PRO:HD3	1.89	0.45
1:D:463:ARG:HG3	1:D:566:ASP:OD2	2.17	0.45
1:E:594:ILE:HG22	1:E:626:GLN:HG3	1.98	0.45
1:A:487:CYS:O	1:A:489:PRO:HD3	2.18	0.44
1:F:447:ILE:O	1:F:450:VAL:HB	2.17	0.44
1:F:728:GLY:O	1:E:728:GLY:HA2	2.17	0.44
1:B:530:LYS:O	1:B:534:LEU:HD23	2.18	0.44
1:D:524:TYR:O	1:D:528:VAL:HG23	2.17	0.44
1:F:506:ASP:O	1:F:508:PRO:HD3	2.18	0.44
1:B:470:THR:O	1:B:501:LYS:HD3	2.18	0.44
1:E:775:LYS:CE	1:E:776:SER:HB2	2.46	0.44
1:C:495:PRO:HD3	1:C:517:HIS:HB2	1.99	0.44
1:B:512:ASP:OD1	1:B:512:ASP:N	2.47	0.44
1:C:519:SER:HA	1:C:524:TYR:CD1	2.53	0.44
1:C:604:GLU:H	1:C:604:GLU:CD	2.21	0.44
1:A:455:ALA:C	1:A:457:ASN:H	2.21	0.44
1:F:444:ARG:HG3	1:F:444:ARG:O	2.17	0.44
1:A:485:LYS:O	1:A:485:LYS:CG	2.66	0.44
1:D:487:CYS:O	1:D:489:PRO:HD3	2.18	0.44
1:B:527:PHE:CE1	1:B:562:GLN:HG3	2.53	0.43
1:D:574:ILE:HG22	1:E:547:ARG:NH2	2.33	0.43
1:D:478:LEU:HA	1:D:481:LEU:HD12	1.99	0.43
1:D:457:ASN:O	1:D:460:GLU:HG2	2.18	0.43
1:C:602:LEU:HD11	1:C:733:ILE:HD12	2.00	0.43
1:E:673:ARG:HG2	1:E:676:LEU:HD12	2.01	0.43
1:A:472:THR:HG23	1:A:476:LYS:HE3	2.00	0.43
1:A:535:GLU:HB3	1:A:540:ILE:HD12	2.00	0.43
1:E:498:VAL:O	1:E:502:ILE:HG13	2.19	0.43
1:E:551:ASP:HA	1:E:552:PRO:HD3	1.90	0.43
1:E:721:TYR:OH	1:E:735:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:PRO:HG2	1:D:570:SER:HB3	2.01	0.43
1:D:673:ARG:HG2	1:D:676:LEU:HD12	2.00	0.43
1:C:756:ILE:O	1:C:760:VAL:HG23	2.18	0.43
1:F:451:HIS:CD2	1:F:485:LYS:HG2	2.54	0.43
1:B:605:ASP:OD1	1:B:605:ASP:N	2.35	0.42
1:F:449:ARG:HH12	1:F:453:ASN:CB	2.11	0.42
1:E:581:ARG:HB3	1:E:582:PRO:HD3	2.01	0.42
1:C:449:ARG:HG2	1:C:765:LEU:HD21	2.02	0.42
1:B:457:ASN:O	1:B:460:GLU:HG2	2.19	0.42
1:A:579:ALA:O	1:A:582:PRO:HD2	2.20	0.42
1:B:478:LEU:HD23	1:B:481:LEU:HD12	2.01	0.42
1:E:478:LEU:HD23	1:E:478:LEU:HA	1.80	0.42
1:D:736:PHE:HE1	1:D:759:SER:HA	1.84	0.42
1:D:766:GLU:O	1:D:770:ILE:CG1	2.53	0.42
1:F:478:LEU:CD1	1:F:491:LEU:HD21	2.50	0.42
1:D:463:ARG:NH1	1:D:563:GLY:O	2.53	0.42
1:D:765:LEU:HD23	1:D:765:LEU:HA	1.88	0.42
1:B:478:LEU:HA	1:B:481:LEU:HD12	2.01	0.42
1:B:642:PRO:HG2	1:B:676:LEU:HD22	2.01	0.42
1:F:481:LEU:HD11	1:F:757:VAL:HA	2.00	0.42
1:E:587:ILE:O	1:E:741:ARG:HD3	2.19	0.42
1:C:495:PRO:O	1:C:499:LYS:HG3	2.20	0.42
1:B:603:LEU:HD11	1:B:608:LEU:HG	2.01	0.42
1:D:729:LYS:HZ1	1:C:729:LYS:HB3	1.52	0.42
1:E:506:ASP:O	1:E:508:PRO:HD3	2.20	0.42
1:A:478:LEU:HA	1:A:478:LEU:HD23	1.79	0.42
1:D:727:ILE:HD12	1:C:601:VAL:HG11	2.01	0.42
1:F:756:ILE:O	1:F:760:VAL:HG23	2.20	0.41
1:E:457:ASN:O	1:E:460:GLU:HG2	2.20	0.41
1:C:634:ILE:O	1:C:637:TYR:HB3	2.20	0.41
1:A:521:HIS:CG	1:A:522:PRO:HD2	2.55	0.41
1:A:769:TYR:O	1:A:773:VAL:HG23	2.20	0.41
1:F:605:ASP:OD1	1:F:605:ASP:N	2.41	0.41
1:E:481:LEU:HD13	1:E:760:VAL:HG11	2.02	0.41
1:C:676:LEU:HD23	1:C:676:LEU:HA	1.83	0.41
1:D:463:ARG:HG3	1:D:463:ARG:H	1.66	0.41
1:C:472:THR:HG23	1:C:476:LYS:HE3	2.01	0.41
1:A:602:LEU:HD11	1:A:733:ILE:HD11	2.01	0.41
1:A:733:ILE:HG22	1:A:736:PHE:HZ	1.84	0.41
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.88	0.41
1:B:519:SER:HA	1:B:524:TYR:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:608:LEU:HD23	1:D:707:ASN:HA	2.02	0.41
1:A:495:PRO:O	1:A:499:LYS:HG3	2.20	0.41
1:F:521:HIS:CG	1:F:522:PRO:HD2	2.55	0.41
1:F:594:ILE:HG22	1:F:626:GLN:HG3	2.02	0.41
1:A:453:ASN:O	1:A:457:ASN:ND2	2.28	0.41
1:D:749:ARG:NH1	1:E:541:ASN:HD22	2.19	0.41
1:E:554:TYR:CE1	1:E:582:PRO:HG3	2.56	0.41
1:C:481:LEU:HD22	1:C:486:ILE:CD1	2.51	0.41
1:A:544:GLU:OE1	1:A:547:ARG:NH2	2.49	0.41
1:A:470:THR:O	1:A:501:LYS:HD3	2.21	0.41
1:B:643:ARG:HB3	1:B:702:LEU:HD11	2.03	0.41
1:E:599:ASN:ND2	1:E:721:TYR:CE1	2.89	0.41
1:C:467:PRO:HG2	1:C:570:SER:HB3	2.03	0.41
1:A:589:VAL:HA	1:A:740:VAL:HA	2.03	0.40
1:B:472:THR:HG23	1:B:476:LYS:HE3	2.03	0.40
1:B:551:ASP:HA	1:B:552:PRO:HD3	1.90	0.40
1:D:636:GLU:OE2	1:D:673:ARG:NH2	2.26	0.40
1:B:597:GLY:HA3	1:B:614:THR:OG1	2.22	0.40
1:C:551:ASP:HA	1:C:552:PRO:HD3	1.84	0.40
1:A:494:TYR:HA	1:A:495:PRO:HD3	1.93	0.40
1:D:647:LEU:O	1:D:662:MET:HG3	2.21	0.40
1:E:729:LYS:HD2	1:E:729:LYS:HA	1.53	0.40
1:B:594:ILE:HG22	1:B:626:GLN:HG3	2.02	0.40
1:C:579:ALA:O	1:C:582:PRO:HD2	2.21	0.40
1:A:551:ASP:HA	1:A:552:PRO:HD3	1.91	0.40
1:D:478:LEU:HD23	1:D:478:LEU:HA	1.88	0.40
1:F:591:LYS:O	1:F:592:GLU:HG2	2.21	0.40
1:F:774:LEU:HD23	1:F:774:LEU:HA	1.78	0.40
1:C:472:THR:CG2	1:C:476:LYS:HE3	2.52	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	336/362 (93%)	332 (99%)	4 (1%)	0	100	100
1	B	336/362 (93%)	330 (98%)	6 (2%)	0	100	100
1	C	337/362 (93%)	333 (99%)	4 (1%)	0	100	100
1	D	336/362 (93%)	329 (98%)	7 (2%)	0	100	100
1	E	336/362 (93%)	332 (99%)	4 (1%)	0	100	100
1	F	336/362 (93%)	331 (98%)	5 (2%)	0	100	100
All	All	2017/2172 (93%)	1987 (98%)	30 (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	282/301 (94%)	280 (99%)	2 (1%)	84	92
1	B	282/301 (94%)	275 (98%)	7 (2%)	47	67
1	C	282/301 (94%)	277 (98%)	5 (2%)	59	76
1	D	282/301 (94%)	270 (96%)	12 (4%)	29	46
1	E	282/301 (94%)	276 (98%)	6 (2%)	53	72
1	F	282/301 (94%)	279 (99%)	3 (1%)	73	87
All	All	1692/1806 (94%)	1657 (98%)	35 (2%)	53	72

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

Mol	Chain	Res	Type
1	A	485	LYS
1	A	771	LYS
1	B	603	LEU
1	B	660	ARG
1	B	721	TYR
1	B	729	LYS
1	B	731	GLU

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Mol	Chain	Res	Type
1	B	772	GLU
1	B	775	LYS
1	D	439	SER
1	D	440	LYS
1	D	441	VAL
1	D	444	ARG
1	D	463	ARG
1	D	482	VAL
1	D	509	LEU
1	D	729	LYS
1	D	731	GLU
1	D	771	LYS
1	D	772	GLU
1	D	775	LYS
1	F	444	ARG
1	F	721	TYR
1	F	771	LYS
1	E	449	ARG
1	E	511	ASN
1	E	606	LYS
1	E	721	TYR
1	E	772	GLU
1	E	775	LYS
1	C	503	LYS
1	C	721	TYR
1	C	727	ILE
1	C	729	LYS
1	C	771	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	338/362 (93%)	0.60	25 (7%) 14 13	53, 72, 99, 114	0
1	B	338/362 (93%)	0.47	15 (4%) 34 33	50, 68, 94, 114	0
1	C	339/362 (93%)	0.55	20 (5%) 22 21	51, 71, 97, 107	0
1	D	338/362 (93%)	0.66	29 (8%) 10 9	55, 74, 107, 129	0
1	E	338/362 (93%)	0.51	14 (4%) 37 36	57, 71, 98, 116	0
1	F	338/362 (93%)	0.69	28 (8%) 11 10	58, 79, 111, 129	0
All	All	2029/2172 (93%)	0.58	131 (6%) 18 17	50, 72, 102, 129	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	LEU	6.0
1	C	509	LEU	5.5
1	F	442	PHE	5.1
1	F	458	GLY	5.0
1	B	486	ILE	4.9
1	F	481	LEU	4.8
1	A	510	LEU	4.4
1	D	502	ILE	4.4
1	F	486	ILE	4.2
1	D	510	LEU	4.1
1	C	494	TYR	4.1
1	E	481	LEU	4.0
1	E	525	PHE	4.0
1	D	747	LEU	4.0
1	D	774	LEU	4.0
1	D	497	ARG	3.9
1	A	727	ILE	3.9
1	A	486	ILE	3.8
1	A	525	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	525	PHE	3.8
1	B	482	VAL	3.8
1	D	509	LEU	3.8
1	F	465	VAL	3.6
1	C	510	LEU	3.6
1	A	529	GLU	3.6
1	D	737	LEU	3.6
1	D	505	LEU	3.5
1	E	761	VAL	3.5
1	B	483	GLU	3.5
1	B	727	ILE	3.4
1	A	762	PHE	3.3
1	F	634	ILE	3.3
1	D	762	PHE	3.3
1	C	481	LEU	3.2
1	D	481	LEU	3.2
1	A	509	LEU	3.2
1	F	608	LEU	3.1
1	D	478	LEU	3.0
1	E	733	ILE	3.0
1	C	507	ILE	3.0
1	C	505	LEU	3.0
1	C	486	ILE	2.9
1	C	762	PHE	2.9
1	C	702	LEU	2.8
1	C	442	PHE	2.8
1	D	727	ILE	2.8
1	F	640	ILE	2.8
1	D	525	PHE	2.8
1	F	507	ILE	2.7
1	C	503	LYS	2.7
1	A	494	TYR	2.7
1	B	507	ILE	2.7
1	F	600	PHE	2.7
1	F	762	PHE	2.7
1	A	531	LEU	2.7
1	A	482	VAL	2.6
1	D	498	VAL	2.6
1	F	491	LEU	2.6
1	F	453	ASN	2.6
1	D	475	LEU	2.6
1	A	637	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	555	PHE	2.5
1	C	634	ILE	2.5
1	F	459	GLY	2.5
1	D	444	ARG	2.5
1	E	762	PHE	2.5
1	A	733	ILE	2.5
1	B	723	LEU	2.5
1	F	602	LEU	2.5
1	F	494	TYR	2.4
1	F	557	ALA	2.4
1	C	733	ILE	2.4
1	A	491	LEU	2.4
1	D	724	ILE	2.4
1	D	584	LEU	2.4
1	F	505	LEU	2.4
1	D	443	ILE	2.3
1	E	486	ILE	2.3
1	A	611	ALA	2.3
1	B	534	LEU	2.3
1	A	454	SER	2.3
1	F	446	ALA	2.3
1	A	601	VAL	2.3
1	D	466	PHE	2.3
1	B	485	LYS	2.2
1	A	569	VAL	2.2
1	F	455	ALA	2.2
1	D	542	LEU	2.2
1	D	442	PHE	2.2
1	B	488	GLN	2.2
1	F	769	TYR	2.2
1	E	678	ILE	2.2
1	A	485	LYS	2.2
1	E	440	LYS	2.2
1	A	507	ILE	2.2
1	A	765	LEU	2.2
1	D	508	PRO	2.2
1	B	469	GLY	2.2
1	B	525	PHE	2.2
1	F	645	ALA	2.2
1	C	608	LEU	2.2
1	C	709	LEU	2.2
1	A	465	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	761	VAL	2.1
1	C	600	PHE	2.1
1	B	461	LEU	2.1
1	D	744	ALA	2.1
1	E	632	ALA	2.1
1	B	594	ILE	2.1
1	F	724	ILE	2.1
1	E	464	ILE	2.1
1	C	727	ILE	2.1
1	D	602	LEU	2.1
1	F	765	LEU	2.1
1	D	494	TYR	2.1
1	C	761	VAL	2.1
1	E	697	PHE	2.1
1	E	555	PHE	2.1
1	F	696	LEU	2.1
1	E	746	VAL	2.1
1	D	491	LEU	2.0
1	F	510	LEU	2.0
1	E	569	VAL	2.0
1	F	638	PHE	2.0
1	B	729	LYS	2.0
1	A	464	ILE	2.0
1	C	706	ALA	2.0
1	D	512	ASP	2.0
1	F	555	PHE	2.0
1	A	483	GLU	2.0
1	A	770	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.