Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2021 – 02:05 am GMT

PDB ID	:	6ZNR
Title	:	MaeB PTA domain R535A mutant
Authors	:	Lovering, A.L.; Harding, C.J.
Deposited on	:	2020-07-06
Resolution	:	2.22 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 ①) were used in the production of this report:

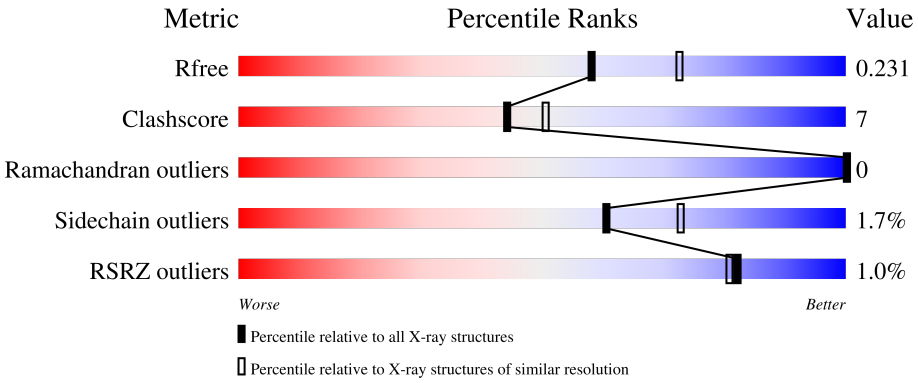
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

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 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	A	362	79% 13% • 7%
1	B	362	78% 14% • 7%
1	C	362	83% 9% • 6%
1	D	362	76% 15% •• 6%
1	E	362	81% 11% • 7%

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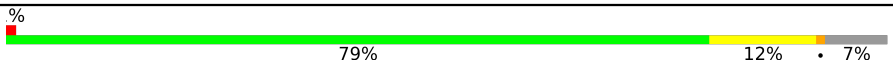
Mol	Chain	Length	Quality of chain
1	F	362	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16005 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
			2592	1655	441	485	11			
1	B	338	Total	C	N	O	S	0	0	0
			2592	1655	441	485	11			
1	D	340	Total	C	N	O	S	0	0	0
			2608	1664	445	488	11			
1	F	338	Total	C	N	O	S	0	0	0
			2592	1655	441	485	11			
1	E	338	Total	C	N	O	S	0	0	0
			2592	1655	441	485	11			
1	C	339	Total	C	N	O	S	0	0	0
			2597	1658	442	486	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	ALA	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	ALA	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	ALA	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	ALA	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	ALA	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	ALA	ARG	engineered mutation	UNP Q6MM15

- Molecule 2 is water.

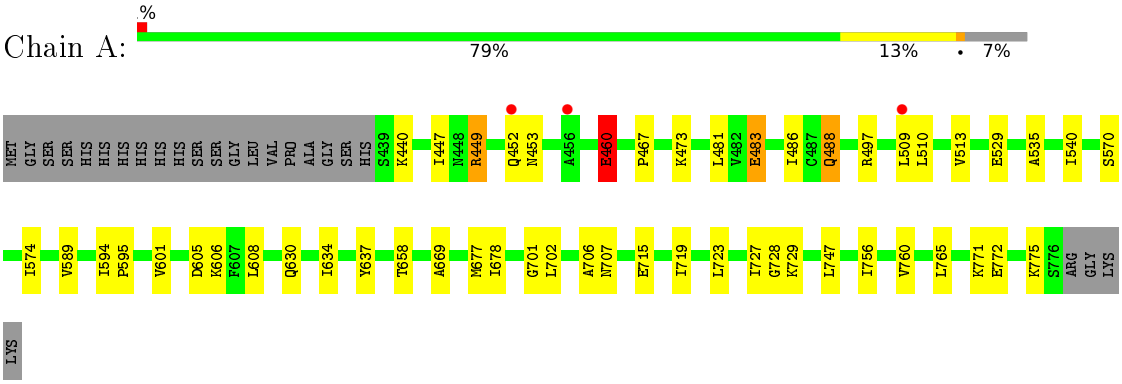
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	62	Total O 62 62	0	0
2	B	97	Total O 97 97	0	0
2	D	54	Total O 54 54	0	0
2	F	58	Total O 58 58	0	0
2	E	69	Total O 69 69	0	0
2	C	92	Total O 92 92	0	0

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.

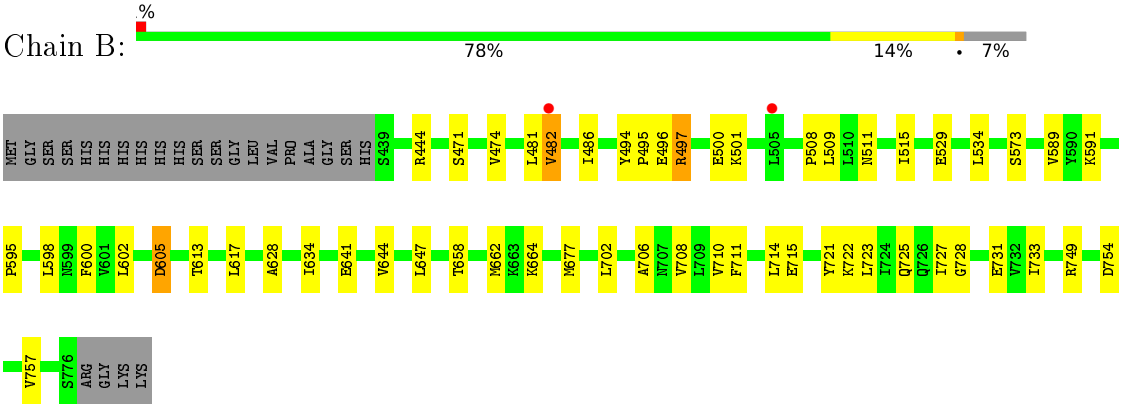
- Molecule 1: Malate dehydrogenase

Chain A:



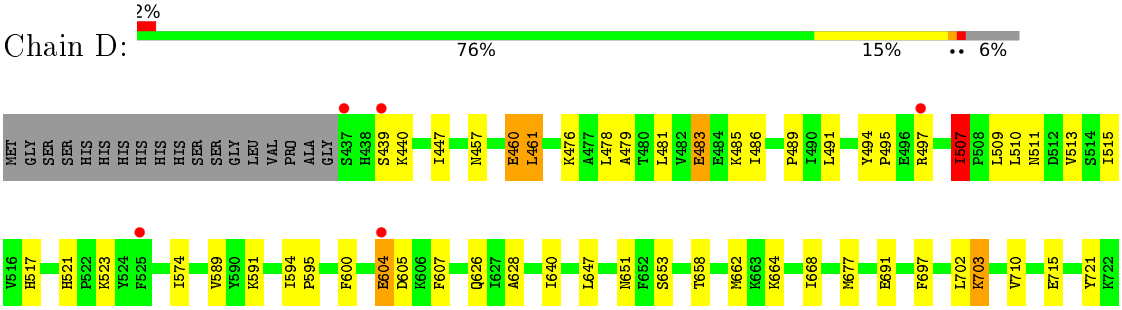
- Molecule 1: Malate dehydrogenase

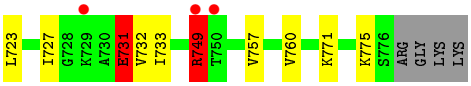
Chain B:



- Molecule 1: Malate dehydrogenase

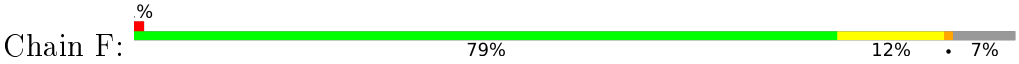
Chain D:

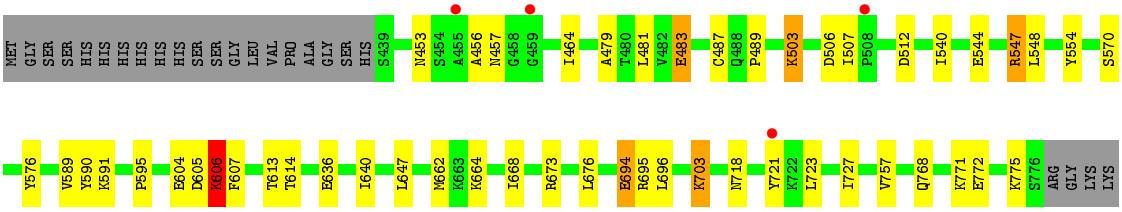




- Molecule 1: Malate dehydrogenase

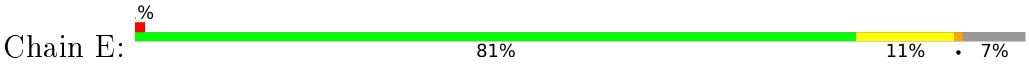
Chain F:

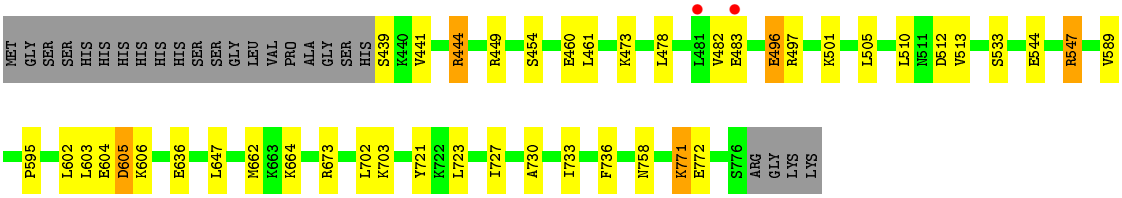




- Molecule 1: Malate dehydrogenase

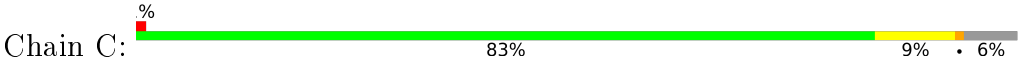
Chain E:

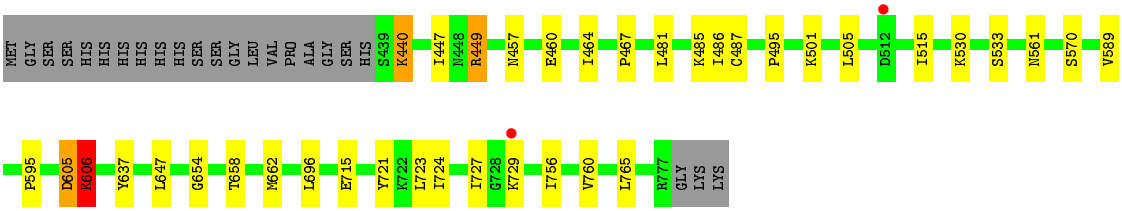




- Molecule 1: Malate dehydrogenase

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.24Å 183.12Å 119.53Å 90.00° 117.08° 90.00°	Depositor
Resolution (Å)	69.41 – 2.22 69.41 – 2.22	Depositor EDS
% Data completeness (in resolution range)	97.8 (69.41-2.22) 98.1 (69.41-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.189 , 0.231 0.190 , 0.231	Depositor DCC
R_{free} test set	6035 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16005	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.51	0/2636	0.73	7/3569 (0.2%)
1	B	0.50	0/2636	0.75	6/3569 (0.2%)
1	C	0.49	1/2641 (0.0%)	0.78	8/3576 (0.2%)
1	D	0.62	6/2653 (0.2%)	0.80	4/3592 (0.1%)
1	E	0.52	1/2636 (0.0%)	0.85	14/3569 (0.4%)
1	F	0.49	1/2636 (0.0%)	0.77	9/3569 (0.3%)
All	All	0.52	9/15838 (0.1%)	0.78	48/21444 (0.2%)

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	B	0	1
1	C	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	461	LEU	C-N	8.22	1.49	1.34
1	D	507	ILE	C-N	8.04	1.49	1.34
1	D	604	GLU	CD-OE1	6.67	1.32	1.25
1	F	694	GLU	CD-OE1	-6.43	1.18	1.25
1	D	591	LYS	CD-CE	6.13	1.66	1.51
1	D	483	GLU	CD-OE1	5.78	1.32	1.25
1	D	771	LYS	CE-NZ	5.70	1.63	1.49
1	E	483	GLU	CD-OE2	5.14	1.31	1.25
1	C	440	LYS	CE-NZ	5.00	1.61	1.49

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	606	LYS	CA-CB-CG	12.62	141.16	113.40
1	E	444	ARG	CA-CB-CG	-9.30	92.94	113.40
1	E	444	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	C	449	ARG	NE-CZ-NH2	8.95	124.77	120.30
1	E	605	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	C	449	ARG	NE-CZ-NH1	-8.37	116.12	120.30
1	E	547	ARG	CG-CD-NE	8.28	129.19	111.80
1	F	703	LYS	CA-CB-CG	-7.92	95.98	113.40
1	E	547	ARG	CA-CB-CG	7.58	130.08	113.40
1	E	547	ARG	CB-CG-CD	-7.58	91.89	111.60
1	D	483	GLU	CA-CB-CG	7.57	130.05	113.40
1	E	483	GLU	CA-CB-CG	-6.93	98.15	113.40
1	F	506	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	C	606	LYS	CB-CG-CD	6.70	129.03	111.60
1	A	473	LYS	CD-CE-NZ	6.69	127.09	111.70
1	B	496	GLU	CA-CB-CG	-6.62	98.85	113.40
1	C	449	ARG	CA-CB-CG	-6.55	98.99	113.40
1	B	444	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	E	496	GLU	N-CA-CB	6.44	122.19	110.60
1	A	483	GLU	CG-CD-OE2	-6.16	105.98	118.30
1	B	605	ASP	CB-CA-C	-6.08	98.25	110.40
1	E	496	GLU	CA-CB-CG	6.07	126.76	113.40
1	F	547	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	488	GLN	CA-CB-CG	5.98	126.56	113.40
1	E	605	ASP	CB-CG-OD1	5.90	123.61	118.30
1	E	444	ARG	CG-CD-NE	-5.88	99.46	111.80
1	F	606	LYS	CB-CA-C	-5.86	98.67	110.40
1	F	694	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	F	512	ASP	CB-CG-OD1	5.76	123.49	118.30
1	C	485	LYS	CD-CE-NZ	5.68	124.77	111.70
1	A	529	GLU	CA-CB-CG	-5.66	100.95	113.40
1	C	606	LYS	CB-CA-C	5.54	121.47	110.40
1	D	749	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	497	ARG	CA-CB-CG	5.35	125.17	113.40
1	F	771	LYS	CB-CG-CD	5.33	125.45	111.60
1	E	604	GLU	N-CA-CB	5.27	120.08	110.60
1	C	729	LYS	CA-CB-CG	5.27	124.98	113.40
1	B	534	LEU	CA-CB-CG	5.21	127.29	115.30
1	F	591	LYS	CD-CE-NZ	5.20	123.66	111.70
1	F	483	GLU	CA-CB-CG	-5.19	101.98	113.40
1	E	771	LYS	CB-CA-C	-5.16	100.08	110.40
1	D	605	ASP	CB-CG-OD1	5.14	122.92	118.30
1	D	731	GLU	CB-CA-C	5.14	120.67	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	483	GLU	CA-CB-CG	5.13	124.70	113.40
1	A	483	GLU	OE1-CD-OE2	5.13	129.46	123.30
1	E	441	VAL	CG1-CB-CG2	5.04	118.97	110.90
1	B	482	VAL	CG1-CB-CG2	5.01	118.92	110.90
1	A	460	GLU	CG-CD-OE2	-5.00	108.30	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	605	ASP	Peptide
1	C	605	ASP	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	2592	0	2665	44	0
1	B	2592	0	2667	35	0
1	C	2597	0	2669	29	0
1	D	2608	0	2677	50	1
1	E	2592	0	2667	27	0
1	F	2592	0	2667	34	0
2	A	62	0	0	0	0
2	B	97	0	0	6	0
2	C	92	0	0	3	0
2	D	54	0	0	0	0
2	E	69	0	0	2	0
2	F	58	0	0	1	0
All	All	16005	0	16012	209	1

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 7.

All (209) 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:479:ALA:O	1:D:483:GLU:OE2	1.52	1.24
1:F:694:GLU:OE1	1:F:703:LYS:HE2	1.58	1.03
1:C:457:ASN:O	1:C:460:GLU:OE1	1.75	1.01
1:C:605:ASP:OD1	1:C:606:LYS:HB3	1.59	1.00
1:F:456:ALA:C	1:F:457:ASN:HD22	1.63	1.00
1:E:544:GLU:OE1	1:E:547:ARG:NH1	1.94	0.99
1:B:529:GLU:OE1	2:B:801:HOH:O	1.89	0.91
1:A:449:ARG:HD2	1:A:765:LEU:HD21	1.55	0.89
1:A:449:ARG:HD2	1:A:765:LEU:CD2	2.04	0.87
1:B:728:GLY:O	2:B:802:HOH:O	1.96	0.84
1:F:456:ALA:O	1:F:457:ASN:ND2	2.11	0.84
1:B:529:GLU:OE2	2:B:803:HOH:O	1.96	0.82
1:A:728:GLY:O	1:A:729:LYS:HD2	1.80	0.80
1:C:658:THR:HG22	2:C:844:HOH:O	1.82	0.79
1:A:483:GLU:OE2	1:A:509:LEU:CD2	2.33	0.77
1:F:456:ALA:C	1:F:457:ASN:ND2	2.39	0.75
1:A:449:ARG:CZ	1:A:453:ASN:HD21	1.91	0.74
1:D:457:ASN:O	1:D:460:GLU:CG	2.37	0.73
1:C:605:ASP:CG	1:C:606:LYS:HB3	2.08	0.72
1:D:479:ALA:O	1:D:483:GLU:CD	2.29	0.71
1:F:694:GLU:OE1	1:F:703:LYS:CE	2.37	0.70
1:D:457:ASN:O	1:D:460:GLU:HG3	1.91	0.69
1:A:460:GLU:H	1:A:460:GLU:CD	1.96	0.69
1:A:728:GLY:C	1:A:729:LYS:HD2	2.14	0.68
1:F:483:GLU:O	1:F:483:GLU:HG3	1.94	0.68
1:A:771:LYS:O	1:A:775:LYS:HG3	1.94	0.68
1:B:481:LEU:HD21	1:B:757:VAL:HG13	1.76	0.67
1:B:725:GLN:OE1	2:B:804:HOH:O	2.11	0.67
1:C:449:ARG:NH2	1:C:637:TYR:CZ	2.62	0.67
1:C:447:ILE:HG23	1:C:486:ILE:HD11	1.79	0.64
1:B:497:ARG:HA	1:B:500:GLU:HG3	1.80	0.63
1:D:439:SER:HB3	1:D:731:GLU:OE1	1.98	0.63
1:C:530:LYS:HE2	1:C:561:ASN:ND2	2.13	0.63
1:D:481:LEU:HD13	1:D:757:VAL:HG22	1.81	0.62
1:F:606:LYS:HB2	1:F:606:LYS:NZ	2.15	0.61
1:D:507:ILE:HD13	1:D:510:LEU:HD12	1.83	0.60
1:F:481:LEU:HD21	1:F:757:VAL:HG13	1.83	0.60
1:E:605:ASP:OD1	1:E:606:LYS:N	2.35	0.60
1:D:489:PRO:HG2	1:D:513:VAL:HG21	1.84	0.60
1:C:654:GLY:O	2:C:802:HOH:O	2.17	0.59
1:B:598:LEU:HD13	1:B:634:ILE:HD12	1.83	0.59
1:E:473:LYS:NZ	2:E:806:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:VAL:HG11	1:B:595:PRO:HD3	1.84	0.59
1:B:602:LEU:HD12	1:B:731:GLU:HG2	1.84	0.59
1:A:449:ARG:HD2	1:A:765:LEU:HD22	1.84	0.59
1:B:471:SER:HB3	1:B:474:VAL:HB	1.85	0.58
1:B:494:TYR:HB2	1:B:497:ARG:HG2	1.84	0.58
1:A:447:ILE:HG23	1:A:486:ILE:HD11	1.84	0.58
1:F:613:THR:HB	1:F:721:TYR:CE2	2.38	0.58
1:A:589:VAL:HG11	1:A:595:PRO:HD3	1.86	0.57
1:A:658:THR:HG21	1:B:715:GLU:OE2	2.04	0.57
1:C:589:VAL:HG11	1:C:595:PRO:HD3	1.85	0.57
1:B:508:PRO:O	1:B:511:ASN:OD1	2.23	0.56
1:D:658:THR:HG21	1:C:715:GLU:OE2	2.05	0.56
1:F:589:VAL:HG12	1:F:590:TYR:O	2.05	0.56
1:E:589:VAL:HG11	1:E:595:PRO:HD3	1.88	0.56
1:A:727:ILE:O	1:A:729:LYS:HE2	2.05	0.56
1:C:530:LYS:HE2	1:C:561:ASN:HD21	1.70	0.55
1:A:574:ILE:HG22	1:F:547:ARG:HH22	1.71	0.55
1:F:772:GLU:O	1:F:775:LYS:HB2	2.07	0.54
1:D:664:LYS:HD3	1:D:668:ILE:HD11	1.88	0.54
1:C:449:ARG:NH2	1:C:637:TYR:CE1	2.75	0.54
1:E:603:LEU:CD1	1:E:606:LYS:HE2	2.37	0.54
1:D:481:LEU:CD2	1:D:760:VAL:HG11	2.38	0.53
1:D:594:ILE:HG22	1:D:626:GLN:HG3	1.90	0.53
1:E:603:LEU:HD12	1:E:606:LYS:HE2	1.90	0.53
1:A:449:ARG:HD3	1:A:453:ASN:ND2	2.24	0.53
1:A:483:GLU:OE2	1:A:509:LEU:HD22	2.08	0.53
1:E:636:GLU:OE2	1:E:673:ARG:NH2	2.26	0.53
1:A:723:LEU:O	1:A:727:ILE:HG12	2.09	0.53
1:D:677:MET:HE3	1:D:702:LEU:HA	1.90	0.52
1:F:607:PHE:CE2	1:F:640:ILE:HD12	2.45	0.52
1:D:607:PHE:CE1	1:D:640:ILE:HD12	2.44	0.52
1:B:482:VAL:HG21	1:B:509:LEU:HB3	1.91	0.52
1:B:495:PRO:HA	1:B:515:ILE:HG21	1.90	0.52
1:A:715:GLU:OE2	1:B:658:THR:HG21	2.10	0.52
1:A:608:LEU:HD23	1:A:707:ASN:HA	1.92	0.52
1:F:589:VAL:HG21	1:F:595:PRO:HD3	1.92	0.52
1:A:772:GLU:O	1:A:775:LYS:HB2	2.10	0.51
1:A:669:ALA:HB1	1:A:678:ILE:HD13	1.92	0.51
1:F:636:GLU:OE2	1:F:673:ARG:NH2	2.36	0.51
1:D:461:LEU:HD11	1:D:485:LYS:CG	2.40	0.51
1:F:718:ASN:HA	1:F:721:TYR:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:LYS:HE2	1:C:505:LEU:HD11	1.93	0.51
1:D:723:LEU:O	1:D:727:ILE:HG12	2.09	0.51
1:D:604:GLU:H	1:D:604:GLU:CD	2.15	0.50
1:A:483:GLU:OE2	1:A:509:LEU:HD21	2.10	0.50
1:E:496:GLU:N	2:E:801:HOH:O	1.97	0.50
1:C:449:ARG:HB3	1:C:765:LEU:HD21	1.92	0.50
1:D:749:ARG:NH2	1:C:696:LEU:HD22	2.26	0.50
1:F:487:CYS:O	1:F:489:PRO:HD3	2.11	0.50
1:C:464:ILE:HG12	1:C:487:CYS:HB2	1.93	0.50
1:D:457:ASN:O	1:D:460:GLU:HG2	2.12	0.49
1:F:481:LEU:HD11	1:F:757:VAL:HA	1.93	0.49
1:F:695:ARG:HB3	1:F:696:LEU:HD12	1.92	0.49
1:F:540:ILE:HA	1:F:544:GLU:OE1	2.13	0.49
1:E:647:LEU:O	1:E:662:MET:HG3	2.13	0.49
1:E:723:LEU:O	1:E:727:ILE:HG12	2.12	0.49
1:E:478:LEU:O	1:E:482:VAL:HG23	2.13	0.49
1:C:467:PRO:HG2	1:C:570:SER:HB3	1.93	0.49
1:C:647:LEU:O	1:C:662:MET:HG3	2.11	0.49
1:F:673:ARG:HG2	1:F:676:LEU:HD12	1.94	0.49
1:B:647:LEU:O	1:B:662:MET:HG3	2.13	0.49
1:B:481:LEU:HD22	1:B:486:ILE:HD11	1.95	0.48
1:D:481:LEU:HD23	1:D:760:VAL:HG11	1.94	0.48
1:C:637:TYR:OH	2:C:801:HOH:O	2.15	0.48
1:A:728:GLY:C	1:A:729:LYS:CD	2.80	0.48
1:D:521:HIS:HE1	1:D:523:LYS:HD2	1.77	0.48
1:E:605:ASP:OD1	1:E:606:LYS:HD3	2.14	0.48
1:C:605:ASP:CG	1:C:606:LYS:CB	2.80	0.48
1:D:600:PHE:O	1:D:732:VAL:HA	2.14	0.48
1:A:630:GLN:O	1:A:634:ILE:HD13	2.14	0.47
1:F:723:LEU:O	1:F:727:ILE:HG12	2.14	0.47
1:D:677:MET:HE1	1:D:703:LYS:O	2.14	0.47
1:B:613:THR:HB	1:B:721:TYR:CE2	2.50	0.47
1:A:449:ARG:HA	1:A:452:GLN:HG2	1.97	0.47
1:E:512:ASP:OD1	1:E:512:ASP:N	2.44	0.47
1:F:647:LEU:O	1:F:662:MET:HG3	2.14	0.47
1:B:644:VAL:HG22	1:B:708:VAL:HB	1.97	0.46
1:B:721:TYR:OH	1:B:722:LYS:HE2	2.15	0.46
1:B:723:LEU:HD22	1:B:727:ILE:HD12	1.97	0.46
1:D:507:ILE:H	1:D:507:ILE:HG13	1.56	0.46
1:A:440:LYS:HE3	1:A:440:LYS:HB2	1.51	0.46
1:A:727:ILE:O	1:A:729:LYS:CD	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:570:SER:HB2	2:F:803:HOH:O	2.14	0.46
1:A:510:LEU:O	1:A:513:VAL:HG12	2.15	0.46
1:D:647:LEU:O	1:D:662:MET:HG3	2.16	0.46
1:B:591:LYS:NZ	2:B:808:HOH:O	2.48	0.46
1:B:494:TYR:HD2	1:B:497:ARG:HE	1.62	0.46
1:A:488:GLN:HE21	1:A:488:GLN:HB3	1.55	0.45
1:A:601:VAL:HB	1:A:608:LEU:HB2	1.98	0.45
1:A:747:LEU:HD13	1:A:756:ILE:HG12	1.98	0.45
1:D:715:GLU:OE2	1:C:658:THR:HG21	2.16	0.45
1:C:481:LEU:HD13	1:C:760:VAL:HG11	1.99	0.45
1:D:628:ALA:HB2	1:D:710:VAL:HG21	1.99	0.45
1:C:756:ILE:O	1:C:760:VAL:HG23	2.16	0.45
1:D:507:ILE:CD1	1:D:510:LEU:HD12	2.46	0.45
1:D:461:LEU:HD11	1:D:485:LYS:HG2	1.99	0.45
1:D:651:ASN:HB3	1:D:697:PHE:CZ	2.52	0.45
1:D:509:LEU:HD12	1:D:509:LEU:HA	1.79	0.45
1:B:509:LEU:HD23	1:B:509:LEU:HA	1.85	0.44
1:F:453:ASN:HB2	1:F:768:GLN:NE2	2.32	0.44
1:F:664:LYS:HD3	1:F:668:ILE:HD11	1.97	0.44
1:E:733:ILE:HG22	1:E:736:PHE:CZ	2.53	0.44
1:A:481:LEU:HD13	1:A:760:VAL:HG11	2.00	0.44
1:A:702:LEU:HD21	1:A:706:ALA:HB2	2.00	0.44
1:E:602:LEU:HD11	1:E:733:ILE:HD11	2.00	0.44
1:B:481:LEU:HD22	1:B:486:ILE:CD1	2.48	0.43
1:B:721:TYR:CZ	1:B:722:LYS:HE2	2.54	0.43
1:C:723:LEU:O	1:C:727:ILE:HG12	2.17	0.43
1:D:439:SER:HB3	1:D:731:GLU:CD	2.38	0.43
1:E:772:GLU:HA	1:E:772:GLU:OE1	2.18	0.43
1:B:702:LEU:HD21	1:B:706:ALA:HB2	2.01	0.43
1:F:676:LEU:HD23	1:F:676:LEU:HA	1.79	0.43
1:E:501:LYS:HE2	1:E:505:LEU:HD11	2.00	0.43
1:A:535:ALA:HB1	1:A:540:ILE:HD12	1.99	0.43
1:A:605:ASP:OD1	1:A:605:ASP:N	2.50	0.43
1:E:454:SER:OG	1:E:461:LEU:HD23	2.19	0.43
1:B:600:PHE:HB2	1:B:733:ILE:CG1	2.48	0.43
1:C:457:ASN:HB3	1:C:460:GLU:OE2	2.19	0.43
1:A:606:LYS:HB3	1:A:606:LYS:HE2	1.85	0.43
1:D:461:LEU:HD11	1:D:485:LYS:HG3	2.01	0.43
1:D:494:TYR:HB2	1:D:497:ARG:CB	2.48	0.43
1:D:447:ILE:HG23	1:D:486:ILE:HD11	2.00	0.42
1:E:605:ASP:OD1	1:E:606:LYS:CG	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:723:LEU:HD23	1:F:723:LEU:HA	1.77	0.42
1:E:733:ILE:HG23	1:E:758:ASN:HB3	2.01	0.42
1:A:449:ARG:CD	1:A:453:ASN:ND2	2.83	0.42
1:E:603:LEU:HD23	1:E:730:ALA:HB2	2.00	0.42
1:C:530:LYS:CE	1:C:561:ASN:ND2	2.82	0.42
1:E:460:GLU:OE2	1:E:771:LYS:HE2	2.20	0.42
1:A:677:MET:HG2	1:A:701:GLY:O	2.19	0.42
1:D:509:LEU:C	1:D:511:ASN:H	2.23	0.42
1:A:594:ILE:HG12	1:A:595:PRO:HD2	2.02	0.42
1:A:608:LEU:CD2	1:A:707:ASN:HA	2.50	0.42
1:D:481:LEU:HD11	1:D:757:VAL:HG13	2.02	0.42
1:D:495:PRO:HA	1:D:515:ILE:HG21	2.02	0.42
1:F:464:ILE:HG12	1:F:487:CYS:HB2	2.01	0.42
1:D:589:VAL:HG11	1:D:595:PRO:HD3	2.00	0.42
1:D:727:ILE:HD11	1:C:724:ILE:HD13	2.02	0.41
1:E:444:ARG:HH11	1:E:444:ARG:HD2	1.45	0.41
1:B:573:SER:HA	1:B:749:ARG:NH1	2.35	0.41
1:D:476:LYS:HB3	1:D:476:LYS:HE2	1.97	0.41
1:D:495:PRO:HD3	1:D:517:HIS:HB2	2.03	0.41
1:D:574:ILE:CG2	1:E:547:ARG:NH2	2.83	0.41
1:A:467:PRO:HG2	1:A:570:SER:HB3	2.00	0.41
1:A:719:ILE:HG21	1:B:711:PHE:CE2	2.55	0.41
1:C:605:ASP:OD1	1:C:605:ASP:N	2.52	0.41
1:E:496:GLU:O	1:E:497:ARG:C	2.59	0.41
1:F:503:LYS:HD2	1:F:503:LYS:C	2.41	0.41
1:F:479:ALA:HB2	1:F:507:ILE:CG2	2.51	0.41
1:E:510:LEU:HD22	1:E:513:VAL:HG21	2.02	0.41
1:B:497:ARG:CZ	2:B:805:HOH:O	2.68	0.41
1:B:617:LEU:HD23	1:B:714:LEU:HD23	2.02	0.41
1:B:628:ALA:HB2	1:B:710:VAL:HG21	2.03	0.41
1:B:641:GLU:OE2	1:B:677:MET:HE2	2.21	0.41
1:D:478:LEU:CD1	1:D:491:LEU:HD21	2.50	0.41
1:F:457:ASN:HD22	1:F:457:ASN:N	2.15	0.41
1:F:548:LEU:O	1:F:554:TYR:HB2	2.21	0.41
1:D:481:LEU:HD21	1:D:760:VAL:HB	2.02	0.41
1:D:440:LYS:N	1:D:440:LYS:HD3	2.34	0.40
1:D:574:ILE:HG21	1:E:547:ARG:NH2	2.35	0.40
1:F:576:TYR:CE1	1:F:614:THR:HB	2.56	0.40
1:A:449:ARG:CD	1:A:765:LEU:HD21	2.40	0.40
1:D:478:LEU:HA	1:D:478:LEU:HD23	1.86	0.40
1:A:449:ARG:NE	1:A:637:TYR:OH	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:494:TYR:HB2	1:D:497:ARG:HB2	2.03	0.40
1:D:600:PHE:HB2	1:D:733:ILE:CG1	2.51	0.40
1:C:495:PRO:HA	1:C:515:ILE:HG21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:775:LYS:NZ	1:D:775:LYS:NZ[2_556]	1.99	0.21

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	Percentiles	
1	A	336/362 (93%)	332 (99%)	4 (1%)	0	100	100
1	B	336/362 (93%)	334 (99%)	2 (1%)	0	100	100
1	C	337/362 (93%)	333 (99%)	4 (1%)	0	100	100
1	D	338/362 (93%)	333 (98%)	5 (2%)	0	100	100
1	E	336/362 (93%)	332 (99%)	4 (1%)	0	100	100
1	F	336/362 (93%)	330 (98%)	6 (2%)	0	100	100
All	All	2019/2172 (93%)	1994 (99%)	25 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	281/300 (94%)	278 (99%)	3 (1%)	73	84
1	B	281/300 (94%)	278 (99%)	3 (1%)	73	84
1	C	281/300 (94%)	277 (99%)	4 (1%)	67	78
1	D	283/300 (94%)	275 (97%)	8 (3%)	43	54
1	E	281/300 (94%)	274 (98%)	7 (2%)	47	58
1	F	281/300 (94%)	277 (99%)	4 (1%)	67	78
All	All	1688/1800 (94%)	1659 (98%)	29 (2%)	60	73

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	449	ARG
1	A	460	GLU
1	A	497	ARG
1	B	501	LYS
1	B	664	LYS
1	B	754	ASP
1	D	460	GLU
1	D	507	ILE
1	D	653	SER
1	D	691	GLU
1	D	703	LYS
1	D	721	TYR
1	D	731	GLU
1	D	749	ARG
1	F	503	LYS
1	F	604	GLU
1	F	605	ASP
1	F	606	LYS
1	E	439	SER
1	E	449	ARG
1	E	533	SER
1	E	664	LYS
1	E	702	LEU
1	E	703	LYS
1	E	721	TYR
1	C	440	LYS
1	C	533	SER

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Mol	Chain	Res	Type
1	C	606	LYS
1	C	721	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	GLN
1	A	453	ASN
1	A	457	ASN
1	A	488	GLN
1	B	511	ASN
1	B	718	ASN
1	D	561	ASN
1	D	562	GLN
1	F	457	ASN
1	F	768	GLN
1	C	561	ASN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	A	338/362 (93%)	-0.10	3 (0%)	84	83	32, 51, 94, 121	0
1	B	338/362 (93%)	-0.21	2 (0%)	89	88	28, 47, 90, 117	0
1	C	339/362 (93%)	-0.17	2 (0%)	89	88	26, 47, 81, 101	0
1	D	340/362 (93%)	0.02	8 (2%)	59	57	29, 57, 104, 144	0
1	E	338/362 (93%)	-0.11	2 (0%)	89	88	30, 51, 94, 108	0
1	F	338/362 (93%)	-0.03	4 (1%)	79	77	34, 59, 104, 125	0
All	All	2031/2172 (93%)	-0.10	21 (1%)	82	81	26, 52, 96, 144	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	456	ALA	5.8
1	D	439	SER	4.3
1	C	729	LYS	4.2
1	D	437	SER	3.5
1	F	455	ALA	3.3
1	D	749	ARG	3.1
1	D	497	ARG	3.0
1	C	512	ASP	2.9
1	D	525	PHE	2.7
1	F	508	PRO	2.6
1	A	509	LEU	2.6
1	A	452	GLN	2.6
1	D	729	LYS	2.5
1	F	721	TYR	2.4
1	D	750	THR	2.3
1	E	483	GLU	2.3
1	F	459	GLY	2.2
1	B	482	VAL	2.2
1	D	604	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	505	LEU	2.1
1	E	481	LEU	2.1

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.