



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:01 AM UTC

PDB ID : 3I6E / pdb_00003i6e
Title : CRYSTAL STRUCTURE OF MUCONATE LACTONIZING ENZYME
FROM *Ruegeria pomeroyi*.
Authors : Fedorov, A.A.; Fedorov, E.V.; Sauder, J.M.; Burley, S.K.; Gerlt, J.A.; Almo,
S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-07-07
Resolution : 1.70 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:

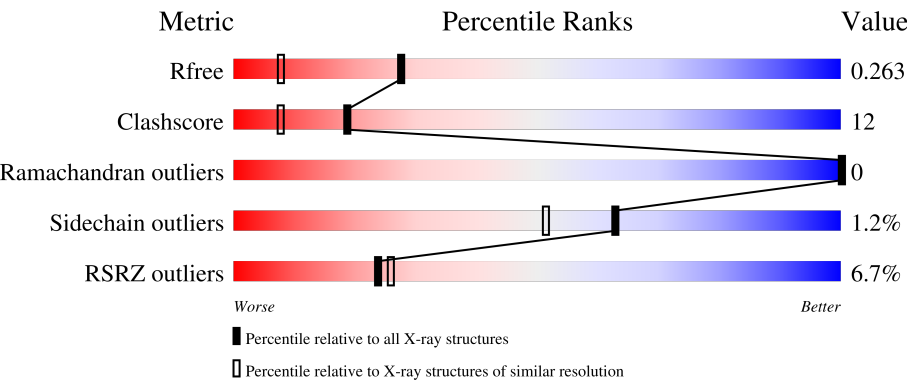
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	385	3% 72%19%8%
1	B	385	5% 74%18%8%
1	C	385	4% 72%19%8%
1	D	385	7% 69%22%8%
1	E	385	11% 69%23%8%

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Mol	Chain	Length	Quality of chain
1	F	385	5% 70% 20% • • 8%
1	G	385	3% 76% 15% • 8%
1	H	385	11% 74% 18% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22777 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 Muconate cycloisomerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2728	1730	480	502	16			
1	B	356	Total	C	N	O	S	0	0	0
			2728	1730	480	502	16			
1	C	356	Total	C	N	O	S	0	0	0
			2728	1730	480	502	16			
1	D	356	Total	C	N	O	S	0	0	0
			2728	1730	480	502	16			
1	E	356	Total	C	N	O	S	0	0	0
			2728	1730	480	502	16			
1	F	356	Total	C	N	O	S	0	0	0
			2728	1730	480	502	16			
1	G	356	Total	C	N	O	S	0	0	0
			2728	1730	480	502	16			
1	H	356	Total	C	N	O	S	0	0	0
			2728	1730	480	502	16			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q5LM96
A	2	SER	-	expression tag	UNP Q5LM96
A	3	LEU	-	expression tag	UNP Q5LM96
A	378	GLU	-	expression tag	UNP Q5LM96
A	379	GLY	-	expression tag	UNP Q5LM96
A	380	HIS	-	expression tag	UNP Q5LM96
A	381	HIS	-	expression tag	UNP Q5LM96
A	382	HIS	-	expression tag	UNP Q5LM96
A	383	HIS	-	expression tag	UNP Q5LM96
A	384	HIS	-	expression tag	UNP Q5LM96
A	385	HIS	-	expression tag	UNP Q5LM96
B	1	MET	-	expression tag	UNP Q5LM96
B	2	SER	-	expression tag	UNP Q5LM96

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	LEU	-	expression tag	UNP Q5LM96
B	378	GLU	-	expression tag	UNP Q5LM96
B	379	GLY	-	expression tag	UNP Q5LM96
B	380	HIS	-	expression tag	UNP Q5LM96
B	381	HIS	-	expression tag	UNP Q5LM96
B	382	HIS	-	expression tag	UNP Q5LM96
B	383	HIS	-	expression tag	UNP Q5LM96
B	384	HIS	-	expression tag	UNP Q5LM96
B	385	HIS	-	expression tag	UNP Q5LM96
C	1	MET	-	expression tag	UNP Q5LM96
C	2	SER	-	expression tag	UNP Q5LM96
C	3	LEU	-	expression tag	UNP Q5LM96
C	378	GLU	-	expression tag	UNP Q5LM96
C	379	GLY	-	expression tag	UNP Q5LM96
C	380	HIS	-	expression tag	UNP Q5LM96
C	381	HIS	-	expression tag	UNP Q5LM96
C	382	HIS	-	expression tag	UNP Q5LM96
C	383	HIS	-	expression tag	UNP Q5LM96
C	384	HIS	-	expression tag	UNP Q5LM96
C	385	HIS	-	expression tag	UNP Q5LM96
D	1	MET	-	expression tag	UNP Q5LM96
D	2	SER	-	expression tag	UNP Q5LM96
D	3	LEU	-	expression tag	UNP Q5LM96
D	378	GLU	-	expression tag	UNP Q5LM96
D	379	GLY	-	expression tag	UNP Q5LM96
D	380	HIS	-	expression tag	UNP Q5LM96
D	381	HIS	-	expression tag	UNP Q5LM96
D	382	HIS	-	expression tag	UNP Q5LM96
D	383	HIS	-	expression tag	UNP Q5LM96
D	384	HIS	-	expression tag	UNP Q5LM96
D	385	HIS	-	expression tag	UNP Q5LM96
E	1	MET	-	expression tag	UNP Q5LM96
E	2	SER	-	expression tag	UNP Q5LM96
E	3	LEU	-	expression tag	UNP Q5LM96
E	378	GLU	-	expression tag	UNP Q5LM96
E	379	GLY	-	expression tag	UNP Q5LM96
E	380	HIS	-	expression tag	UNP Q5LM96
E	381	HIS	-	expression tag	UNP Q5LM96
E	382	HIS	-	expression tag	UNP Q5LM96
E	383	HIS	-	expression tag	UNP Q5LM96
E	384	HIS	-	expression tag	UNP Q5LM96
E	385	HIS	-	expression tag	UNP Q5LM96

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	expression tag	UNP Q5LM96
F	2	SER	-	expression tag	UNP Q5LM96
F	3	LEU	-	expression tag	UNP Q5LM96
F	378	GLU	-	expression tag	UNP Q5LM96
F	379	GLY	-	expression tag	UNP Q5LM96
F	380	HIS	-	expression tag	UNP Q5LM96
F	381	HIS	-	expression tag	UNP Q5LM96
F	382	HIS	-	expression tag	UNP Q5LM96
F	383	HIS	-	expression tag	UNP Q5LM96
F	384	HIS	-	expression tag	UNP Q5LM96
F	385	HIS	-	expression tag	UNP Q5LM96
G	1	MET	-	expression tag	UNP Q5LM96
G	2	SER	-	expression tag	UNP Q5LM96
G	3	LEU	-	expression tag	UNP Q5LM96
G	378	GLU	-	expression tag	UNP Q5LM96
G	379	GLY	-	expression tag	UNP Q5LM96
G	380	HIS	-	expression tag	UNP Q5LM96
G	381	HIS	-	expression tag	UNP Q5LM96
G	382	HIS	-	expression tag	UNP Q5LM96
G	383	HIS	-	expression tag	UNP Q5LM96
G	384	HIS	-	expression tag	UNP Q5LM96
G	385	HIS	-	expression tag	UNP Q5LM96
H	1	MET	-	expression tag	UNP Q5LM96
H	2	SER	-	expression tag	UNP Q5LM96
H	3	LEU	-	expression tag	UNP Q5LM96
H	378	GLU	-	expression tag	UNP Q5LM96
H	379	GLY	-	expression tag	UNP Q5LM96
H	380	HIS	-	expression tag	UNP Q5LM96
H	381	HIS	-	expression tag	UNP Q5LM96
H	382	HIS	-	expression tag	UNP Q5LM96
H	383	HIS	-	expression tag	UNP Q5LM96
H	384	HIS	-	expression tag	UNP Q5LM96
H	385	HIS	-	expression tag	UNP Q5LM96

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0
2	G	1	Total 1	Mg 1	0	0
2	H	1	Total 1	Mg 1	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0
3	E	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0
3	G	1	Total 1	Na 1	0	0
3	H	1	Total 1	Na 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total 125	O 125	0	0
4	B	133	Total 133	O 133	0	0
4	C	97	Total 97	O 97	0	0
4	D	116	Total 116	O 116	0	0

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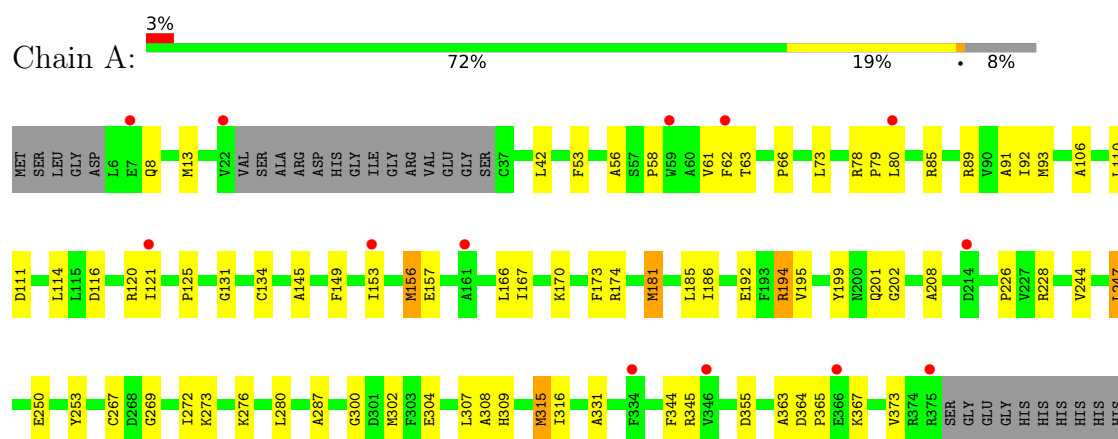
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	101	Total 101	O 101	0	0
4	F	130	Total 130	O 130	0	0
4	G	150	Total 150	O 150	0	0
4	H	85	Total 85	O 85	0	0

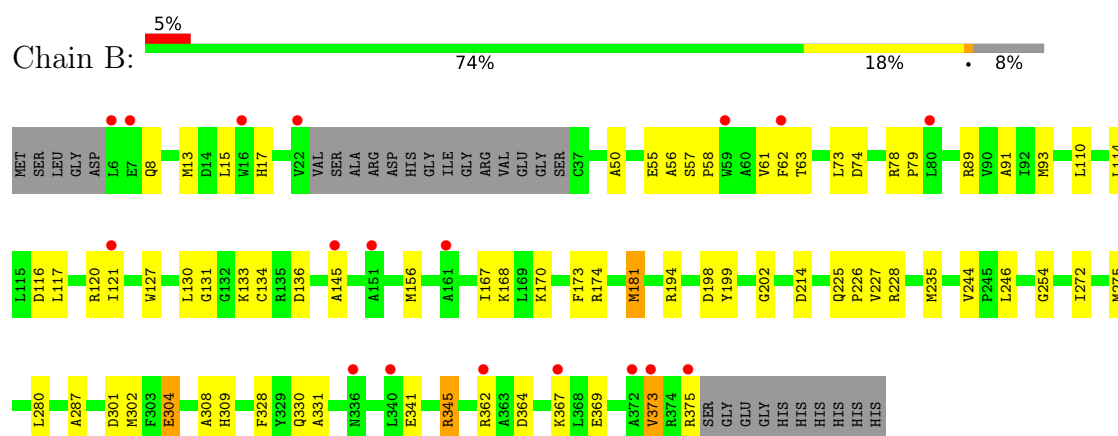
3 Residue-property plots [i](#)

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.

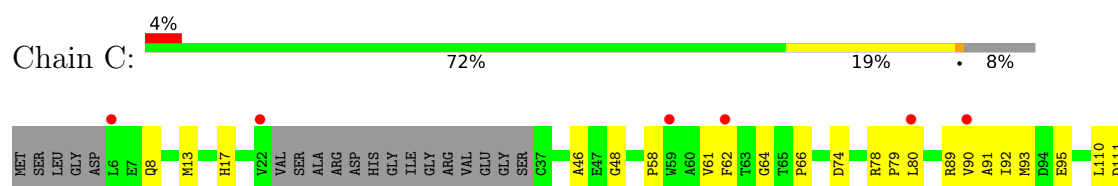
• Molecule 1: Muconate cycloisomerase I



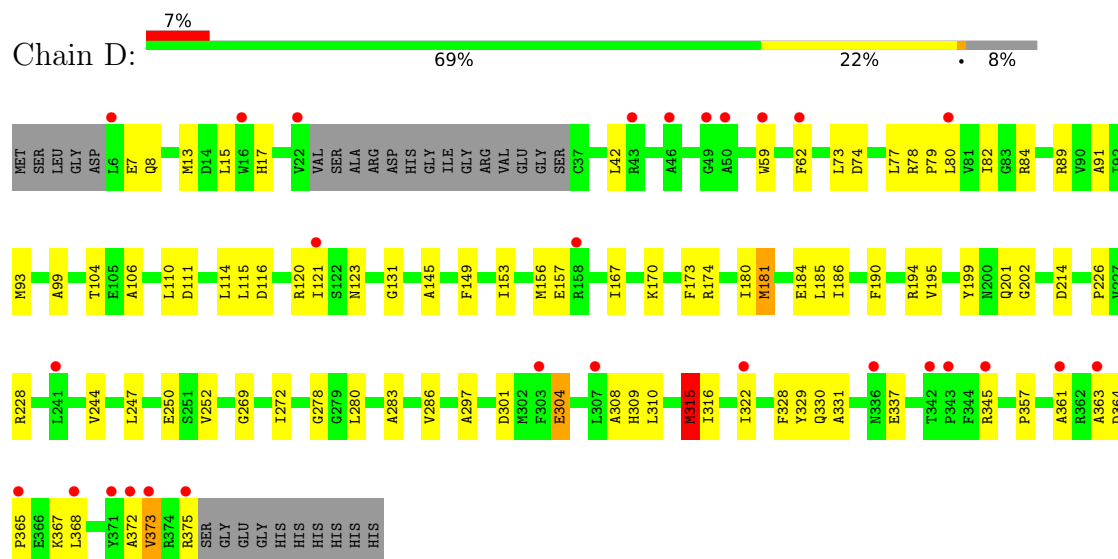
• Molecule 1: Muconate cycloisomerase I



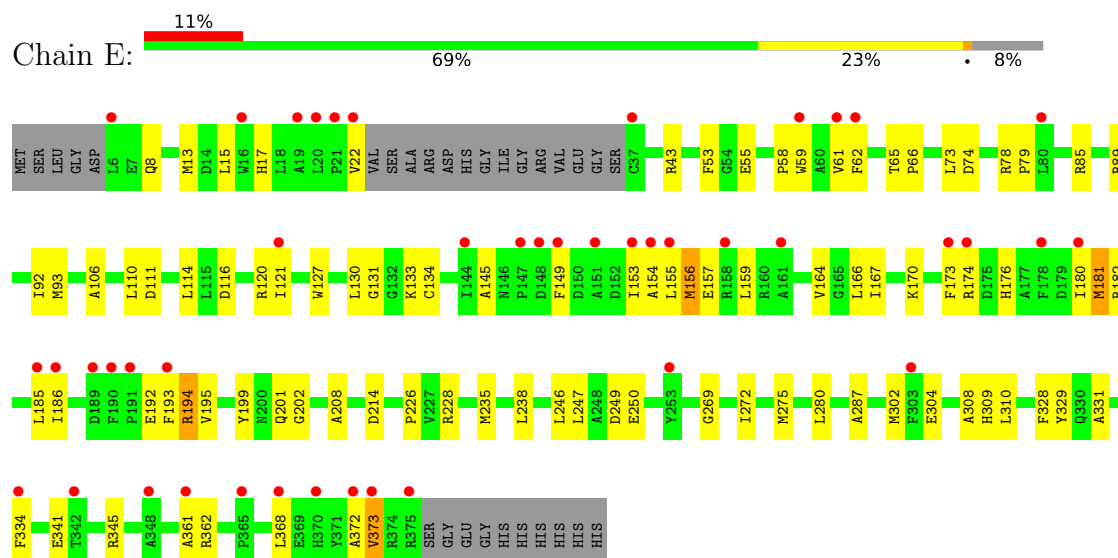
• Molecule 1: Muconate cycloisomerase I



- Molecule 1: Muconate cycloisomerase I

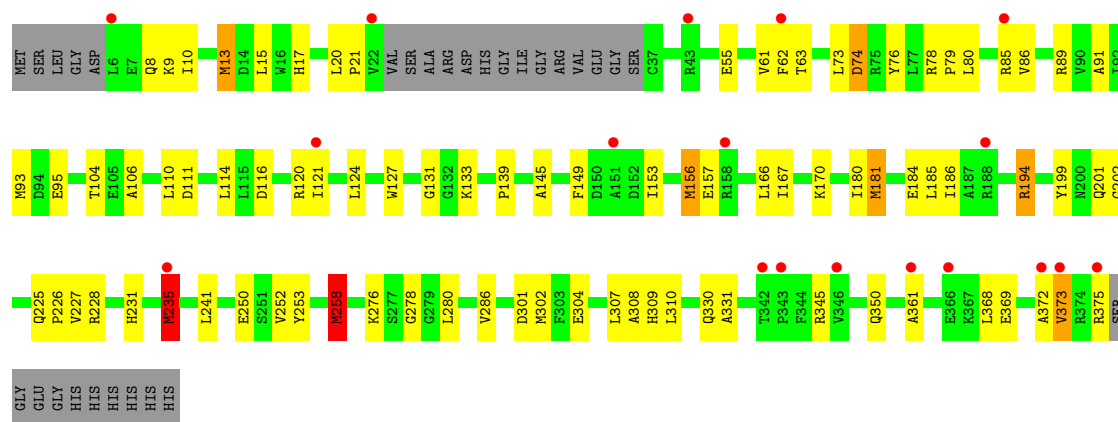


- Molecule 1: Muconate cycloisomerase I

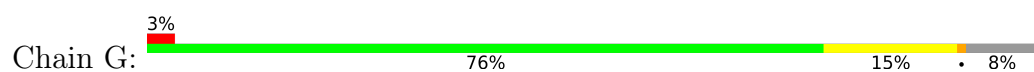


- Molecule 1: Muconate cycloisomerase I

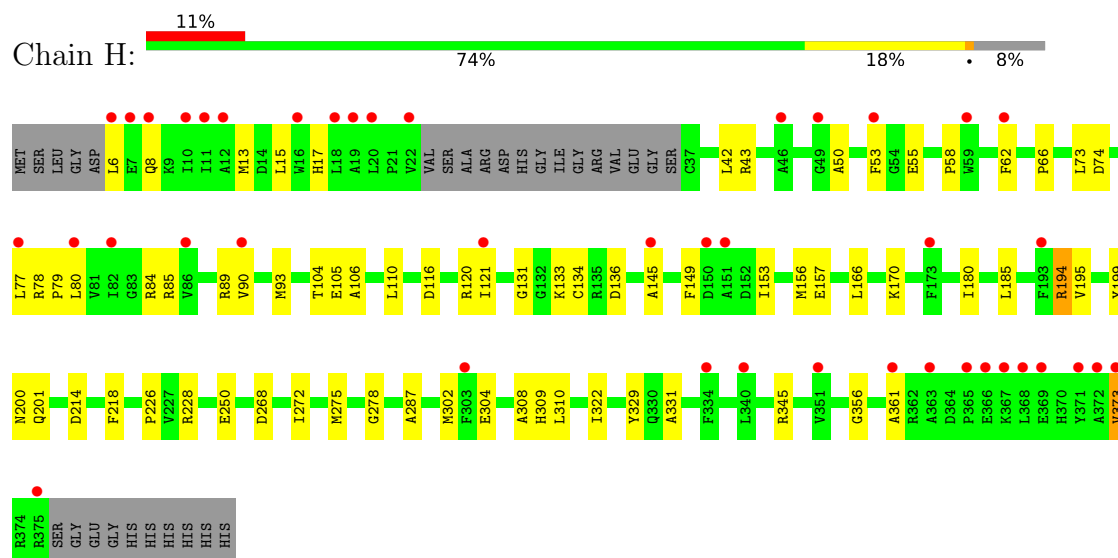




• Molecule 1: Muconate cycloisomerase I



• Molecule 1: Muconate cycloisomerase I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.14Å 135.36Å 113.02Å 90.00° 103.18° 90.00°	Depositor
Resolution (Å)	24.87 – 1.70 24.87 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (24.87-1.70) 97.8 (24.87-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.263 0.234 , 0.263	Depositor DCC
R_{free} test set	17364 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22777	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: NA, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	1/2782 (0.0%)	0.94	9/3773 (0.2%)
1	B	0.41	0/2782	0.93	8/3773 (0.2%)
1	C	0.38	0/2782	0.92	10/3773 (0.3%)
1	D	0.43	1/2782 (0.0%)	0.94	9/3773 (0.2%)
1	E	0.41	1/2782 (0.0%)	0.90	6/3773 (0.2%)
1	F	0.51	5/2782 (0.2%)	0.95	9/3773 (0.2%)
1	G	0.47	2/2782 (0.1%)	0.95	9/3773 (0.2%)
1	H	0.39	1/2782 (0.0%)	0.90	7/3773 (0.2%)
All	All	0.43	11/22256 (0.0%)	0.93	67/30184 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	315	MET	SD-CE	-8.84	1.57	1.79
1	F	235	MET	CB-CG	8.41	1.77	1.52
1	G	275	MET	SD-CE	-8.20	1.59	1.79
1	F	156	MET	SD-CE	-7.83	1.59	1.79
1	G	156	MET	SD-CE	-7.06	1.61	1.79
1	H	156	MET	SD-CE	-6.79	1.62	1.79
1	F	13	MET	SD-CE	-6.29	1.63	1.79
1	F	258	MET	SD-CE	-5.97	1.64	1.79
1	E	156	MET	SD-CE	-5.42	1.66	1.79
1	F	235	MET	CG-SD	-5.15	1.67	1.80
1	A	156	MET	SD-CE	-5.12	1.66	1.79

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	202	GLY	N-CA-C	8.58	124.54	114.16
1	E	194	ARG	N-CA-C	-8.52	95.78	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ARG	N-CA-C	-8.20	96.31	109.76
1	B	194	ARG	N-CA-C	-8.15	96.27	109.96
1	B	202	GLY	N-CA-C	8.09	124.35	113.99
1	D	194	ARG	N-CA-C	-7.95	96.61	109.96
1	H	194	ARG	N-CA-C	-7.88	96.72	109.96
1	F	194	ARG	N-CA-C	-7.82	96.83	109.96
1	G	194	ARG	N-CA-C	-7.69	97.04	109.96
1	G	345	ARG	N-CA-C	7.68	120.89	109.59
1	B	373	VAL	N-CA-C	-7.68	105.06	113.43
1	C	194	ARG	N-CA-C	-7.53	96.97	109.24
1	D	202	GLY	N-CA-C	7.43	122.84	114.67
1	H	373	VAL	N-CA-C	-7.42	105.34	113.43
1	F	202	GLY	N-CA-C	7.26	122.66	114.67
1	B	345	ARG	N-CA-C	7.23	120.22	109.59
1	C	345	ARG	N-CA-C	7.21	120.19	109.59
1	C	202	GLY	N-CA-C	7.07	122.45	114.67
1	H	345	ARG	N-CA-C	7.04	119.93	109.59
1	F	345	ARG	N-CA-C	6.99	119.86	109.59
1	A	202	GLY	N-CA-C	6.99	122.36	114.67
1	C	373	VAL	N-CA-C	-6.92	105.89	113.43
1	F	373	VAL	N-CA-C	-6.91	105.89	113.43
1	A	345	ARG	N-CA-C	6.90	119.73	109.59
1	G	373	VAL	N-CA-C	-6.71	104.97	113.22
1	E	373	VAL	N-CA-C	-6.70	106.47	112.90
1	D	345	ARG	N-CA-C	6.67	119.90	109.96
1	G	244	VAL	N-CA-C	-6.48	103.06	108.63
1	E	345	ARG	N-CA-C	6.41	119.01	109.59
1	D	195	VAL	N-CA-C	6.34	117.05	108.17
1	A	244	VAL	N-CA-C	-6.22	103.28	108.63
1	D	373	VAL	N-CA-C	-6.12	107.16	113.10
1	E	202	GLY	N-CA-C	6.12	121.57	114.16
1	F	235	MET	N-CA-C	-6.03	104.82	111.82
1	D	330	GLN	N-CA-C	5.98	117.80	111.28
1	D	244	VAL	N-CA-C	-5.70	103.73	108.63
1	D	252	VAL	N-CA-C	5.58	116.62	107.24
1	B	254	GLY	CA-C-N	5.58	125.25	119.05
1	B	254	GLY	C-N-CA	5.58	125.25	119.05
1	H	195	VAL	N-CA-C	5.57	115.97	108.17
1	E	208	ALA	N-CA-C	5.54	117.01	110.97
1	A	208	ALA	N-CA-C	5.54	117.00	111.07
1	C	252	VAL	N-CA-C	5.51	116.50	107.24
1	F	330	GLN	N-CA-C	5.50	117.28	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	CYS	N-CA-C	5.47	116.28	108.74
1	G	74	ASP	N-CA-C	5.46	117.23	111.28
1	A	195	VAL	N-CA-C	5.38	115.70	108.17
1	C	244	VAL	N-CA-C	-5.32	104.06	108.63
1	F	241	LEU	N-CA-C	5.30	119.47	112.89
1	C	208	ALA	N-CA-C	5.28	116.73	110.97
1	F	74	ASP	N-CA-C	5.26	116.70	111.07
1	H	268	ASP	N-CA-C	-5.20	106.96	113.72
1	B	244	VAL	N-CA-C	-5.20	104.16	108.63
1	G	195	VAL	N-CA-C	5.15	115.38	108.17
1	A	344	PHE	N-CA-C	-5.14	101.74	109.15
1	C	268	ASP	N-CA-C	-5.13	107.05	113.72
1	A	267	CYS	N-CA-C	5.12	116.07	108.60
1	H	356	GLY	CA-C-N	5.11	125.02	119.76
1	H	356	GLY	C-N-CA	5.11	125.02	119.76
1	A	373	VAL	N-CA-C	-5.09	106.96	113.22
1	D	7	GLU	N-CA-C	-5.09	107.03	113.18
1	F	76	TYR	N-CA-C	5.07	119.50	112.45
1	C	74	ASP	N-CA-C	5.07	116.81	111.28
1	B	330	GLN	N-CA-C	5.06	116.79	111.28
1	G	342	THR	CA-C-N	5.04	125.04	119.90
1	G	342	THR	C-N-CA	5.04	125.04	119.90
1	E	195	VAL	N-CA-C	5.01	115.79	108.53

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	2728	0	2719	57	0
1	B	2728	0	2719	63	0
1	C	2728	0	2719	66	0
1	D	2728	0	2719	76	0
1	E	2728	0	2719	80	0
1	F	2728	0	2719	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2728	0	2719	56	0
1	H	2728	0	2719	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	125	0	0	1	0
4	B	133	0	0	2	0
4	C	97	0	0	1	0
4	D	116	0	0	1	0
4	E	101	0	0	1	0
4	F	130	0	0	2	0
4	G	150	0	0	1	0
4	H	85	0	0	1	0
All	All	22777	0	21752	520	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 12.

All (520) 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:F:235:MET:CG	1:F:235:MET:CB	1.77	1.60
1:G:57:SER:H	1:G:275:MET:HE2	1.03	1.15
1:F:93:MET:HE2	1:F:93:MET:HA	1.40	1.04
1:F:227:VAL:H	1:F:235:MET:HE1	1.36	0.91
1:G:57:SER:H	1:G:275:MET:CE	1.83	0.90
1:G:181:MET:HE2	1:G:181:MET:O	1.72	0.90
1:H:93:MET:HE2	1:H:93:MET:HA	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:ALA:HB1	1:G:170:LYS:HD3	1.55	0.88
1:E:226:PRO:HD2	1:E:235:MET:HE1	1.55	0.88
1:G:56:ALA:HA	1:G:275:MET:HE1	1.56	0.88
1:F:225:GLN:NE2	1:F:235:MET:HE2	1.89	0.87
1:F:252:VAL:HG11	1:F:258:MET:HE3	1.57	0.86
1:F:227:VAL:HG13	4:F:392:HOH:O	1.75	0.86
1:D:8:GLN:HE22	1:D:121:ILE:HD12	1.38	0.86
1:G:57:SER:N	1:G:275:MET:HE2	1.88	0.86
1:B:227:VAL:HG22	1:B:235:MET:HE2	1.55	0.86
1:D:283:ALA:O	1:D:286:VAL:HG22	1.77	0.85
1:A:181:MET:HE2	1:A:181:MET:O	1.79	0.83
1:F:8:GLN:HE22	1:F:121:ILE:HD12	1.44	0.82
1:B:225:GLN:NE2	1:B:235:MET:HE3	1.95	0.81
1:D:93:MET:HE1	1:D:110:LEU:CD2	2.11	0.81
1:B:227:VAL:CG2	1:B:235:MET:HE2	2.10	0.80
1:F:93:MET:HE1	1:F:110:LEU:HD23	1.62	0.79
1:D:181:MET:HE2	1:D:181:MET:O	1.83	0.79
1:A:131:GLY:HA2	1:B:89:ARG:HH21	1.48	0.79
1:H:93:MET:HE1	1:H:110:LEU:HD23	1.64	0.78
1:G:156:MET:HE3	1:G:167:ILE:HD13	1.66	0.78
1:A:93:MET:HE1	1:A:110:LEU:CD2	2.13	0.77
1:G:309:HIS:HE1	1:G:331:ALA:H	1.32	0.77
1:E:93:MET:HE1	1:E:110:LEU:CD2	2.13	0.77
1:F:227:VAL:H	1:F:235:MET:CE	1.98	0.77
1:C:93:MET:HE1	1:C:110:LEU:HG	1.65	0.77
1:F:227:VAL:N	1:F:235:MET:HE1	1.99	0.77
1:B:93:MET:HE1	1:B:110:LEU:CD2	2.14	0.76
1:C:93:MET:HE1	1:C:110:LEU:CD2	2.15	0.76
1:B:93:MET:HE2	1:B:93:MET:HA	1.66	0.76
1:D:13:MET:HE1	1:D:74:ASP:HA	1.66	0.76
1:D:13:MET:HE2	1:D:78:ARG:NH2	2.00	0.76
1:F:63:THR:HG21	1:F:302:MET:HE3	1.67	0.76
1:E:13:MET:HE2	1:E:78:ARG:CZ	2.16	0.75
1:G:13:MET:HE2	1:G:78:ARG:NH2	2.01	0.75
1:B:116:ASP:O	1:B:120:ARG:HG2	1.87	0.74
1:F:258:MET:HA	1:F:258:MET:HE2	1.68	0.74
1:F:258:MET:HG3	1:F:286:VAL:HG13	1.70	0.73
1:G:13:MET:HE1	1:G:74:ASP:HA	1.69	0.73
1:H:13:MET:HE2	1:H:78:ARG:CZ	2.18	0.73
1:F:258:MET:CG	1:F:286:VAL:HG13	2.19	0.73
1:B:228:ARG:HG2	4:B:393:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:MET:HE1	1:B:110:LEU:HD23	1.71	0.72
1:F:225:GLN:HA	1:F:235:MET:HE3	1.70	0.72
1:G:13:MET:HE2	1:G:78:ARG:CZ	2.20	0.71
1:D:272:ILE:HD13	1:D:286:VAL:HG23	1.71	0.71
1:G:13:MET:HE3	1:G:15:LEU:HD11	1.72	0.71
1:E:226:PRO:HD2	1:E:235:MET:CE	2.21	0.71
1:E:153:ILE:O	1:E:157:GLU:HG2	1.91	0.70
1:C:309:HIS:HE1	1:C:331:ALA:H	1.36	0.70
1:E:156:MET:HE3	1:E:167:ILE:HD13	1.72	0.70
1:A:315:MET:HG3	1:A:316:ILE:N	2.06	0.69
1:E:304:GLU:HB2	1:E:308:ALA:HB3	1.75	0.69
1:A:156:MET:HE3	1:A:167:ILE:HD13	1.73	0.69
1:A:181:MET:HE2	1:A:181:MET:C	2.18	0.69
1:F:227:VAL:O	1:F:235:MET:HE1	1.93	0.69
1:A:309:HIS:HE1	1:A:331:ALA:H	1.39	0.69
1:D:8:GLN:NE2	1:D:121:ILE:HD12	2.09	0.68
1:G:8:GLN:HE22	1:G:121:ILE:HD12	1.56	0.68
1:D:93:MET:HE1	1:D:110:LEU:HD23	1.75	0.68
1:E:228:ARG:HG2	4:E:388:HOH:O	1.93	0.68
1:H:93:MET:HE1	1:H:110:LEU:CD2	2.24	0.68
1:E:309:HIS:HE1	1:E:331:ALA:H	1.40	0.68
1:H:8:GLN:HE22	1:H:121:ILE:HD12	1.59	0.68
1:C:93:MET:HE1	1:C:110:LEU:CG	2.23	0.68
1:D:93:MET:HE2	1:D:93:MET:HA	1.74	0.68
1:E:235:MET:HE3	1:E:235:MET:HA	1.75	0.68
1:A:89:ARG:HH21	1:B:131:GLY:HA2	1.60	0.67
1:C:8:GLN:HE21	1:C:46:ALA:HB1	1.60	0.67
1:C:275:MET:HB2	1:C:302:MET:HE2	1.76	0.66
1:E:78:ARG:HB3	1:E:79:PRO:HD3	1.76	0.66
1:E:85:ARG:HH11	1:E:85:ARG:HG3	1.60	0.66
1:C:304:GLU:HB2	1:C:308:ALA:HB3	1.78	0.66
1:H:153:ILE:O	1:H:157:GLU:HG2	1.96	0.66
1:F:227:VAL:HG12	1:F:228:ARG:N	2.10	0.66
1:E:58:PRO:HG3	1:E:66:PRO:HA	1.77	0.65
1:E:235:MET:HE2	1:E:246:LEU:HD21	1.77	0.65
1:F:93:MET:HA	1:F:93:MET:CE	2.24	0.65
1:B:13:MET:HE3	1:B:15:LEU:HD11	1.79	0.65
1:F:201:GLN:NE2	1:F:250:GLU:HG2	2.12	0.65
1:D:78:ARG:HB3	1:D:79:PRO:HD3	1.79	0.64
1:F:13:MET:HE1	1:F:74:ASP:HA	1.78	0.64
1:F:131:GLY:O	1:H:90:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:ALA:CB	1:G:170:LYS:HD3	2.27	0.64
1:F:145:ALA:HB1	1:F:170:LYS:HD3	1.79	0.64
1:C:180:ILE:O	1:C:184:GLU:HG3	1.98	0.63
1:B:173:PHE:CD1	1:B:174:ARG:HG3	2.34	0.63
1:B:309:HIS:HE1	1:B:331:ALA:H	1.45	0.63
1:C:58:PRO:HG3	1:C:66:PRO:HA	1.81	0.63
1:E:93:MET:HE1	1:E:110:LEU:HG	1.80	0.63
1:E:176:HIS:NE2	1:E:180:ILE:HD11	2.14	0.62
1:A:228:ARG:HG2	4:A:425:HOH:O	1.98	0.62
1:F:13:MET:HE2	1:F:78:ARG:NH2	2.14	0.62
1:E:235:MET:HE3	1:E:238:LEU:HD12	1.81	0.62
1:H:13:MET:HE1	1:H:74:ASP:HA	1.80	0.62
1:A:304:GLU:HB2	1:A:308:ALA:HB3	1.82	0.62
1:C:213:LEU:HD21	1:C:241:LEU:HB3	1.81	0.62
1:H:13:MET:HE2	1:H:78:ARG:NH2	2.14	0.62
1:E:181:MET:C	1:E:181:MET:HE2	2.24	0.62
1:F:89:ARG:HH21	1:H:131:GLY:HA2	1.64	0.62
1:F:309:HIS:HE1	1:F:331:ALA:H	1.48	0.62
1:C:181:MET:O	1:C:181:MET:HE2	1.99	0.62
1:F:78:ARG:HB3	1:F:79:PRO:HD3	1.82	0.62
1:G:181:MET:HE2	1:G:181:MET:C	2.24	0.62
1:F:252:VAL:HG21	1:F:258:MET:CE	2.30	0.61
1:F:304:GLU:HB2	1:F:308:ALA:HB3	1.82	0.61
1:C:116:ASP:O	1:C:120:ARG:HG2	2.00	0.61
1:D:116:ASP:O	1:D:120:ARG:HG2	2.01	0.61
1:F:13:MET:HE2	1:F:78:ARG:CZ	2.30	0.61
1:D:309:HIS:HE1	1:D:331:ALA:H	1.46	0.61
1:C:201:GLN:NE2	1:C:250:GLU:HG2	2.16	0.61
1:A:247:LEU:HD22	1:A:269:GLY:C	2.26	0.61
1:G:116:ASP:O	1:G:120:ARG:HG2	2.02	0.60
1:H:13:MET:HE1	1:H:73:LEU:O	2.00	0.60
1:F:80:LEU:HD11	1:F:95:GLU:OE1	2.01	0.60
1:D:131:GLY:O	1:G:90:VAL:HG23	2.01	0.60
1:D:272:ILE:HD12	1:D:322:ILE:HD11	1.84	0.60
1:E:181:MET:HE2	1:E:181:MET:O	2.02	0.59
1:A:93:MET:HE1	1:A:110:LEU:HG	1.83	0.59
1:E:310:LEU:HD11	1:E:361:ALA:HB3	1.84	0.59
1:H:309:HIS:HE1	1:H:331:ALA:H	1.49	0.59
1:A:78:ARG:HB3	1:A:79:PRO:HD3	1.83	0.59
1:E:341:GLU:HG3	1:E:362:ARG:O	2.02	0.59
1:H:304:GLU:HB2	1:H:308:ALA:HB3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:MET:HE1	1:B:74:ASP:HA	1.85	0.59
1:B:89:ARG:HG3	1:B:114:LEU:HD13	1.85	0.59
1:C:274:ILE:HG13	1:C:275:MET:HE2	1.85	0.59
1:E:93:MET:HE1	1:E:110:LEU:CG	2.33	0.59
1:B:369:GLU:OE2	1:B:375:ARG:NE	2.35	0.59
1:C:93:MET:HE3	1:C:114:LEU:CD1	2.31	0.59
1:G:13:MET:HE3	1:G:15:LEU:CD1	2.33	0.59
1:G:304:GLU:HB2	1:G:308:ALA:HB3	1.84	0.59
1:D:149:PHE:HE2	1:D:185:LEU:HD13	1.67	0.59
1:C:90:VAL:HG23	1:E:131:GLY:O	2.03	0.59
1:D:78:ARG:O	1:D:82:ILE:HD13	2.03	0.59
1:C:149:PHE:HE2	1:C:185:LEU:HD13	1.66	0.59
1:E:199:TYR:HB2	1:E:226:PRO:HA	1.85	0.58
1:H:116:ASP:O	1:H:120:ARG:HG2	2.03	0.58
1:F:180:ILE:O	1:F:184:GLU:HG3	2.02	0.58
1:E:93:MET:HE1	1:E:110:LEU:HD23	1.83	0.58
1:B:8:GLN:HE22	1:B:121:ILE:HD12	1.67	0.58
1:C:127:TRP:CH2	1:C:133:LYS:HD2	2.38	0.58
1:E:61:VAL:HG23	1:E:62:PHE:CD1	2.38	0.58
1:B:127:TRP:CZ2	1:B:133:LYS:HD2	2.38	0.58
1:D:272:ILE:HD12	1:D:322:ILE:CD1	2.33	0.58
1:F:181:MET:HE2	1:F:181:MET:O	2.04	0.58
1:A:93:MET:HE1	1:A:110:LEU:HD23	1.85	0.58
1:F:127:TRP:CZ2	1:F:133:LYS:HD2	2.39	0.58
1:G:8:GLN:NE2	1:G:121:ILE:HD12	2.18	0.58
1:F:116:ASP:O	1:F:120:ARG:HG2	2.03	0.58
1:B:63:THR:HG21	1:B:302:MET:HE3	1.84	0.57
1:E:173:PHE:CD1	1:E:174:ARG:HG3	2.39	0.57
1:H:272:ILE:HD12	1:H:322:ILE:HD11	1.85	0.57
1:E:93:MET:HA	1:E:93:MET:HE2	1.85	0.57
1:C:93:MET:HE3	1:C:114:LEU:HD12	1.86	0.57
1:D:156:MET:HE1	1:D:186:ILE:HG12	1.86	0.57
1:F:156:MET:HE3	1:F:167:ILE:HD13	1.86	0.57
1:G:364:ASP:HB3	1:G:367:LYS:HG3	1.86	0.57
1:A:201:GLN:NE2	1:A:250:GLU:HG2	2.20	0.57
1:E:127:TRP:CZ2	1:E:133:LYS:HD2	2.39	0.57
1:H:13:MET:CE	1:H:74:ASP:HA	2.34	0.57
1:B:364:ASP:OD2	1:B:367:LYS:HG3	2.03	0.57
1:A:93:MET:HE2	1:A:93:MET:HA	1.87	0.57
1:C:228:ARG:HG2	4:C:616:HOH:O	2.05	0.57
1:F:93:MET:HE1	1:F:110:LEU:CD2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:GLN:NE2	1:C:48:GLY:H	2.03	0.57
1:D:13:MET:HE2	1:D:78:ARG:CZ	2.34	0.57
1:D:145:ALA:HB1	1:D:170:LYS:HD3	1.87	0.57
1:D:315:MET:HE3	1:D:316:ILE:HG12	1.87	0.57
1:A:93:MET:HE1	1:A:110:LEU:CG	2.34	0.56
1:C:89:ARG:HG3	1:C:114:LEU:HD13	1.87	0.56
1:C:156:MET:HE3	1:C:167:ILE:HD13	1.88	0.56
1:B:156:MET:HE3	1:B:167:ILE:HD13	1.88	0.56
1:C:89:ARG:HH21	1:E:131:GLY:HA2	1.71	0.56
1:C:93:MET:CE	1:C:110:LEU:HG	2.35	0.56
1:E:13:MET:HE2	1:E:78:ARG:NH2	2.20	0.56
1:H:145:ALA:HB1	1:H:170:LYS:HD3	1.88	0.56
1:B:345:ARG:HG2	1:B:345:ARG:HH11	1.70	0.56
1:E:149:PHE:CE2	1:E:181:MET:HE1	2.41	0.56
1:E:185:LEU:HD23	1:E:185:LEU:C	2.31	0.56
1:C:145:ALA:HB1	1:C:170:LYS:HD3	1.87	0.56
1:F:89:ARG:HG3	1:F:114:LEU:HD13	1.88	0.55
1:D:337:GLU:CD	1:D:367:LYS:HE2	2.32	0.55
1:B:13:MET:HE2	1:B:78:ARG:NH2	2.22	0.55
1:B:61:VAL:HG23	1:B:62:PHE:CD1	2.41	0.55
1:C:80:LEU:HD11	1:C:95:GLU:OE1	2.06	0.55
1:A:173:PHE:CD1	1:A:174:ARG:HG3	2.42	0.55
1:E:247:LEU:HD22	1:E:269:GLY:C	2.31	0.55
1:D:173:PHE:CD1	1:D:174:ARG:HG3	2.41	0.55
1:E:13:MET:HE1	1:E:73:LEU:O	2.06	0.55
1:B:181:MET:HE2	1:B:181:MET:O	2.07	0.55
1:F:8:GLN:NE2	1:F:121:ILE:HD12	2.17	0.55
1:G:105:GLU:HB3	1:G:275:MET:CE	2.36	0.54
1:A:80:LEU:C	1:A:80:LEU:HD12	2.32	0.54
1:H:272:ILE:HD12	1:H:322:ILE:CD1	2.38	0.54
1:C:185:LEU:C	1:C:185:LEU:HD23	2.33	0.54
1:D:156:MET:HE3	1:D:167:ILE:HD13	1.89	0.54
1:B:93:MET:HE1	1:B:110:LEU:CG	2.37	0.54
1:E:120:ARG:NH2	1:E:362:ARG:HG3	2.22	0.54
1:H:201:GLN:NE2	1:H:250:GLU:HG2	2.23	0.54
1:C:274:ILE:HG13	1:C:275:MET:CE	2.37	0.54
1:B:8:GLN:NE2	1:B:121:ILE:HD12	2.23	0.54
1:D:364:ASP:HB3	1:D:367:LYS:CG	2.38	0.54
1:F:153:ILE:O	1:F:157:GLU:HG2	2.07	0.54
1:F:227:VAL:CG1	1:F:228:ARG:N	2.71	0.54
1:G:201:GLN:NE2	1:G:250:GLU:HG2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:LEU:HD21	1:D:99:ALA:HB2	1.90	0.53
1:H:228:ARG:HG2	4:H:391:HOH:O	2.09	0.53
1:B:93:MET:HE1	1:B:110:LEU:HG	1.89	0.53
1:B:227:VAL:H	1:B:235:MET:CE	2.21	0.53
1:E:13:MET:HE1	1:E:74:ASP:HA	1.91	0.53
1:G:73:LEU:HG	1:G:106:ALA:HB1	1.90	0.53
1:B:78:ARG:N	1:B:79:PRO:HD2	2.23	0.53
1:C:363:ALA:O	1:C:365:PRO:HD3	2.09	0.53
1:D:199:TYR:HB2	1:D:226:PRO:HA	1.90	0.53
1:D:228:ARG:HG2	4:D:567:HOH:O	2.09	0.53
1:B:55:GLU:O	1:B:275:MET:HE1	2.09	0.52
1:D:13:MET:HG3	1:D:42:LEU:HD11	1.91	0.52
1:D:91:ALA:HB2	1:G:134:CYS:HA	1.92	0.52
1:G:149:PHE:CE2	1:G:181:MET:HE1	2.44	0.52
1:B:362:ARG:HG3	1:B:362:ARG:HH11	1.75	0.52
1:D:131:GLY:HA2	1:G:89:ARG:HH21	1.74	0.52
1:H:73:LEU:HG	1:H:106:ALA:HB1	1.92	0.52
1:A:93:MET:HE3	1:A:114:LEU:CD1	2.40	0.52
1:D:363:ALA:O	1:D:365:PRO:HD3	2.09	0.52
1:D:89:ARG:NH1	1:D:111:ASP:OD1	2.43	0.52
1:D:272:ILE:CD1	1:D:286:VAL:HG23	2.38	0.52
1:E:17:HIS:O	1:E:373:VAL:HG22	2.10	0.52
1:E:201:GLN:NE2	1:E:250:GLU:HG2	2.23	0.52
1:F:89:ARG:HH21	1:H:131:GLY:CA	2.23	0.52
1:C:61:VAL:HG23	1:C:62:PHE:CD1	2.45	0.52
1:D:93:MET:HE2	1:D:93:MET:CA	2.40	0.52
1:F:225:GLN:HE21	1:F:235:MET:HE2	1.71	0.52
1:A:149:PHE:CE2	1:A:181:MET:HE1	2.45	0.51
1:C:309:HIS:CE1	1:C:331:ALA:H	2.24	0.51
1:A:145:ALA:HB1	1:A:170:LYS:HD3	1.92	0.51
1:C:156:MET:HE1	1:C:186:ILE:HG12	1.93	0.51
1:D:283:ALA:O	1:D:286:VAL:CG2	2.55	0.51
1:F:225:GLN:CA	1:F:235:MET:HE3	2.38	0.51
1:B:227:VAL:HG23	1:B:235:MET:HE2	1.93	0.51
1:F:55:GLU:HB2	1:F:307:LEU:HD23	1.92	0.51
1:F:13:MET:HE3	1:F:15:LEU:HD11	1.93	0.51
1:G:13:MET:CE	1:G:15:LEU:HD11	2.41	0.51
1:H:50:ALA:HB3	1:H:121:ILE:HD11	1.93	0.51
1:B:304:GLU:HB2	1:B:308:ALA:HB3	1.92	0.50
1:D:185:LEU:C	1:D:185:LEU:HD23	2.36	0.50
1:F:124:LEU:HD21	1:H:6:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:ARG:HG2	4:F:392:HOH:O	2.10	0.50
1:H:199:TYR:HB2	1:H:226:PRO:HA	1.94	0.50
1:G:247:LEU:HD22	1:G:269:GLY:C	2.36	0.50
1:G:272:ILE:CD1	1:G:287:ALA:HB2	2.41	0.50
1:H:93:MET:HE2	1:H:93:MET:CA	2.35	0.50
1:A:156:MET:HE1	1:A:186:ILE:HG12	1.92	0.50
1:C:91:ALA:HB2	1:E:134:CYS:HA	1.93	0.50
1:F:61:VAL:HG23	1:F:62:PHE:CD1	2.47	0.50
1:D:304:GLU:HB2	1:D:308:ALA:HB3	1.94	0.50
1:H:185:LEU:C	1:H:185:LEU:HD23	2.37	0.50
1:A:125:PRO:HG3	1:A:355:ASP:O	2.12	0.50
1:C:17:HIS:O	1:C:373:VAL:HG22	2.11	0.50
1:C:92:ILE:HG22	1:C:93:MET:HE2	1.94	0.50
1:C:199:TYR:HB2	1:C:226:PRO:HA	1.94	0.50
1:G:180:ILE:O	1:G:184:GLU:HG3	2.12	0.50
1:H:13:MET:HE3	1:H:15:LEU:HD11	1.94	0.49
1:A:280:LEU:HD12	1:A:280:LEU:N	2.27	0.49
1:C:149:PHE:CE2	1:C:185:LEU:HD13	2.47	0.49
1:D:73:LEU:HG	1:D:106:ALA:HB1	1.94	0.49
1:E:149:PHE:HE2	1:E:185:LEU:HD13	1.77	0.49
1:H:85:ARG:HG3	1:H:85:ARG:HH11	1.77	0.49
1:B:309:HIS:CE1	1:B:331:ALA:H	2.29	0.49
1:D:13:MET:CE	1:D:74:ASP:HA	2.37	0.49
1:B:17:HIS:O	1:B:373:VAL:HG22	2.12	0.49
1:F:149:PHE:HE2	1:F:185:LEU:HD13	1.77	0.49
1:F:368:LEU:O	1:F:372:ALA:HB2	2.13	0.49
1:F:199:TYR:HB2	1:F:226:PRO:HA	1.94	0.49
1:F:310:LEU:HD11	1:F:361:ALA:HB3	1.95	0.49
1:F:304:GLU:HG3	1:F:309:HIS:CD2	2.48	0.49
1:A:8:GLN:NE2	1:A:121:ILE:HD12	2.28	0.49
1:D:315:MET:HG3	1:D:316:ILE:N	2.27	0.49
1:E:73:LEU:HG	1:E:106:ALA:HB1	1.95	0.49
1:F:235:MET:CB	1:F:235:MET:SD	2.90	0.48
1:D:93:MET:HE1	1:D:110:LEU:CG	2.43	0.48
1:G:105:GLU:HA	1:G:275:MET:HE3	1.95	0.48
1:A:363:ALA:O	1:A:365:PRO:HD3	2.13	0.48
1:G:127:TRP:CZ2	1:G:133:LYS:HD2	2.48	0.48
1:G:156:MET:HE1	1:G:186:ILE:HG12	1.94	0.48
1:H:78:ARG:N	1:H:79:PRO:HD2	2.28	0.48
1:B:13:MET:CE	1:B:15:LEU:HD11	2.43	0.48
1:C:173:PHE:CD1	1:C:174:ARG:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ASN:ND2	1:D:357:PRO:HG3	2.28	0.48
1:F:258:MET:HG2	1:F:286:VAL:HG13	1.92	0.48
1:H:55:GLU:O	1:H:275:MET:HE1	2.14	0.48
1:F:280:LEU:N	1:F:280:LEU:HD12	2.28	0.48
1:C:13:MET:HB3	1:C:78:ARG:NH1	2.28	0.48
1:A:58:PRO:HG2	1:A:66:PRO:HA	1.96	0.48
1:A:272:ILE:CD1	1:A:287:ALA:HB2	2.44	0.48
1:D:149:PHE:CE2	1:D:185:LEU:HD13	2.47	0.48
1:G:302:MET:O	1:G:304:GLU:HG2	2.13	0.48
1:D:309:HIS:CE1	1:D:331:ALA:H	2.31	0.48
1:D:73:LEU:HD23	1:D:77:LEU:HD12	1.96	0.48
1:D:82:ILE:HD12	1:D:82:ILE:N	2.29	0.48
1:F:252:VAL:HG11	1:F:258:MET:CE	2.36	0.48
1:H:80:LEU:O	1:H:84:ARG:HG3	2.14	0.47
1:E:166:LEU:HD23	1:E:194:ARG:HB2	1.96	0.47
1:G:156:MET:HE2	1:G:193:PHE:CE2	2.49	0.47
1:H:58:PRO:HB3	1:H:105:GLU:OE2	2.14	0.47
1:B:93:MET:CE	1:B:110:LEU:HG	2.45	0.47
1:C:272:ILE:CD1	1:C:287:ALA:HB2	2.44	0.47
1:D:368:LEU:O	1:D:372:ALA:HB2	2.14	0.47
1:E:192:GLU:CD	1:E:192:GLU:H	2.21	0.47
1:D:59:TRP:HD1	1:D:62:PHE:CD2	2.32	0.47
1:E:8:GLN:HE22	1:E:121:ILE:HD12	1.80	0.47
1:E:85:ARG:HG3	1:E:85:ARG:NH1	2.29	0.47
1:F:9:LYS:HZ3	1:F:85:ARG:NH1	2.11	0.47
1:D:297:ALA:CB	1:D:322:ILE:HD13	2.44	0.47
1:E:302:MET:O	1:E:304:GLU:HG2	2.15	0.47
1:E:309:HIS:CG	1:E:328:PHE:HB3	2.50	0.47
1:C:89:ARG:NH2	1:E:131:GLY:HA2	2.28	0.47
1:F:227:VAL:CG1	1:F:228:ARG:H	2.27	0.47
1:G:309:HIS:CE1	1:G:331:ALA:H	2.21	0.47
1:H:309:HIS:CE1	1:H:331:ALA:H	2.30	0.47
1:A:93:MET:CE	1:A:110:LEU:HG	2.45	0.47
1:B:145:ALA:HB1	1:B:170:LYS:HD3	1.96	0.47
1:B:227:VAL:H	1:B:235:MET:HE1	1.79	0.47
1:C:93:MET:HE1	1:C:110:LEU:HD23	1.95	0.47
1:D:309:HIS:CG	1:D:328:PHE:HB3	2.50	0.47
1:H:133:LYS:HD3	1:H:136:ASP:OD1	2.15	0.47
1:A:73:LEU:HG	1:A:106:ALA:HB1	1.96	0.47
1:B:56:ALA:C	1:B:58:PRO:HD3	2.40	0.47
1:C:133:LYS:HB2	1:C:133:LYS:HZ2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ILE:HD11	1:F:86:VAL:HG22	1.96	0.46
1:F:252:VAL:HG21	1:F:258:MET:HE3	1.97	0.46
1:B:50:ALA:HB3	1:B:121:ILE:HD11	1.97	0.46
1:B:117:LEU:O	1:B:121:ILE:HG12	2.15	0.46
1:C:89:ARG:NH1	1:C:111:ASP:OD1	2.49	0.46
1:F:131:GLY:HA2	1:H:89:ARG:NH2	2.30	0.46
1:G:78:ARG:N	1:G:79:PRO:HD2	2.30	0.46
1:D:13:MET:HE3	1:D:15:LEU:HD11	1.97	0.46
1:D:247:LEU:HD22	1:D:269:GLY:C	2.40	0.46
1:E:145:ALA:HB1	1:E:170:LYS:HD3	1.97	0.46
1:E:176:HIS:HE2	1:E:180:ILE:HD11	1.80	0.46
1:G:105:GLU:HB3	1:G:275:MET:HE3	1.97	0.46
1:G:199:TYR:HB2	1:G:226:PRO:HA	1.98	0.46
1:A:131:GLY:HA2	1:B:89:ARG:NH2	2.23	0.46
1:C:192:GLU:CD	1:C:192:GLU:H	2.24	0.46
1:G:59:TRP:HD1	1:G:62:PHE:CD2	2.33	0.46
1:H:58:PRO:HG3	1:H:66:PRO:HA	1.98	0.46
1:A:63:THR:HG21	1:A:302:MET:HE3	1.97	0.46
1:F:17:HIS:O	1:F:373:VAL:HG22	2.15	0.46
1:G:56:ALA:C	1:G:58:PRO:HD3	2.41	0.46
1:E:93:MET:CE	1:E:110:LEU:HG	2.44	0.46
1:F:252:VAL:HG11	1:F:258:MET:HG2	1.98	0.46
1:B:131:GLY:N	4:B:424:HOH:O	2.44	0.45
1:B:225:GLN:HE21	1:B:235:MET:HE3	1.75	0.45
1:A:85:ARG:HH11	1:A:85:ARG:HG2	1.81	0.45
1:F:185:LEU:C	1:F:185:LEU:HD23	2.41	0.45
1:C:133:LYS:HE3	1:C:136:ASP:OD1	2.16	0.45
1:E:173:PHE:CE1	1:E:174:ARG:HG3	2.52	0.45
1:G:105:GLU:CB	1:G:275:MET:HE3	2.46	0.45
1:G:228:ARG:HG2	4:G:395:HOH:O	2.16	0.45
1:A:149:PHE:HE2	1:A:181:MET:HE1	1.81	0.45
1:B:280:LEU:N	1:B:280:LEU:HD12	2.31	0.45
1:E:55:GLU:O	1:E:275:MET:HE1	2.17	0.45
1:E:130:LEU:HD11	1:E:280:LEU:HD23	1.97	0.45
1:F:227:VAL:CG1	1:F:231:HIS:CD2	3.00	0.45
1:C:58:PRO:HB2	1:C:64:GLY:O	2.17	0.45
1:G:61:VAL:HG23	1:G:62:PHE:CD1	2.52	0.45
1:G:156:MET:HE2	1:G:193:PHE:HE2	1.82	0.45
1:B:199:TYR:HB2	1:B:226:PRO:HA	1.99	0.45
1:E:272:ILE:CD1	1:E:287:ALA:HB2	2.47	0.45
1:E:309:HIS:CE1	1:E:331:ALA:H	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:PHE:CZ	1:H:250:GLU:HG3	2.51	0.45
1:B:93:MET:HE2	1:B:93:MET:CA	2.42	0.45
1:F:89:ARG:NH1	1:F:111:ASP:OD1	2.47	0.45
1:E:65:THR:HB	1:E:66:PRO:HD2	1.99	0.45
1:H:272:ILE:CD1	1:H:287:ALA:HB2	2.46	0.45
1:B:272:ILE:CD1	1:B:287:ALA:HB2	2.47	0.45
1:E:93:MET:HE3	1:E:114:LEU:CD1	2.47	0.45
1:E:164:VAL:O	1:E:193:PHE:HE1	1.99	0.45
1:F:139:PRO:HA	1:F:350:GLN:NE2	2.31	0.45
1:A:89:ARG:NH2	1:B:131:GLY:HA2	2.28	0.44
1:E:22:VAL:HG11	1:E:334:PHE:CE2	2.52	0.44
1:H:17:HIS:O	1:H:373:VAL:HG22	2.17	0.44
1:E:8:GLN:NE2	1:E:121:ILE:HD12	2.32	0.44
1:H:15:LEU:HD12	1:H:74:ASP:HB2	1.98	0.44
1:H:73:LEU:HD23	1:H:77:LEU:HD12	2.00	0.44
1:H:310:LEU:HD11	1:H:361:ALA:HB3	1.99	0.44
1:B:309:HIS:CG	1:B:328:PHE:HB3	2.53	0.44
1:D:59:TRP:CD1	1:D:62:PHE:CD2	3.06	0.44
1:D:93:MET:HE1	1:D:110:LEU:HG	1.98	0.44
1:E:59:TRP:HD1	1:E:62:PHE:CD2	2.35	0.44
1:F:139:PRO:HA	1:F:350:GLN:HE22	1.83	0.44
1:H:93:MET:HA	1:H:93:MET:CE	2.36	0.44
1:C:8:GLN:HE21	1:C:46:ALA:CB	2.29	0.44
1:A:131:GLY:CA	1:B:89:ARG:HH21	2.25	0.44
1:A:199:TYR:HB2	1:A:226:PRO:HA	1.98	0.44
1:B:13:MET:HE1	1:B:73:LEU:C	2.43	0.44
1:H:62:PHE:CZ	1:H:250:GLU:HA	2.53	0.44
1:H:287:ALA:HB2	1:H:322:ILE:HD11	2.00	0.43
1:H:302:MET:O	1:H:304:GLU:HG2	2.17	0.43
1:A:364:ASP:OD2	1:A:367:LYS:HG3	2.18	0.43
1:C:133:LYS:NZ	1:C:133:LYS:CB	2.80	0.43
1:C:156:MET:HE1	1:C:186:ILE:HG23	2.00	0.43
1:D:93:MET:HE3	1:D:114:LEU:CD1	2.48	0.43
1:G:375:ARG:HG2	1:G:375:ARG:HH11	1.82	0.43
1:F:201:GLN:NE2	1:F:250:GLU:CG	2.80	0.43
1:D:17:HIS:O	1:D:373:VAL:HG22	2.18	0.43
1:F:166:LEU:HD23	1:F:194:ARG:HB2	1.99	0.43
1:F:10:ILE:CD1	1:F:86:VAL:HG22	2.48	0.43
1:F:13:MET:HE1	1:F:73:LEU:O	2.18	0.43
1:C:329:TYR:CD1	1:C:329:TYR:C	2.96	0.43
1:D:180:ILE:O	1:D:184:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:ALA:O	1:E:157:GLU:HB2	2.19	0.43
1:G:166:LEU:HD23	1:G:194:ARG:HB2	2.01	0.43
1:A:134:CYS:HA	1:B:91:ALA:HB2	2.00	0.43
1:H:180:ILE:HD12	1:H:218:PHE:HE2	1.84	0.43
1:C:78:ARG:N	1:C:79:PRO:HD2	2.33	0.43
1:C:131:GLY:HA2	1:E:89:ARG:NH2	2.34	0.43
1:C:131:GLY:HA2	1:E:89:ARG:HH21	1.84	0.42
1:D:80:LEU:O	1:D:84:ARG:HG3	2.18	0.42
1:D:310:LEU:HD11	1:D:361:ALA:HB3	2.01	0.42
1:E:89:ARG:NH1	1:E:111:ASP:OD1	2.49	0.42
1:G:280:LEU:N	1:G:280:LEU:HD12	2.33	0.42
1:H:166:LEU:HD23	1:H:194:ARG:HB2	2.01	0.42
1:H:13:MET:HG3	1:H:42:LEU:HD11	2.00	0.42
1:A:56:ALA:C	1:A:58:PRO:HD3	2.44	0.42
1:D:315:MET:HE3	1:D:316:ILE:CG1	2.49	0.42
1:F:91:ALA:HB2	1:H:134:CYS:HA	2.01	0.42
1:F:227:VAL:HG12	1:F:228:ARG:H	1.78	0.42
1:A:273:LYS:HG2	1:A:300:GLY:C	2.45	0.42
1:D:375:ARG:HH11	1:D:375:ARG:HG2	1.83	0.42
1:E:280:LEU:HD12	1:E:280:LEU:N	2.34	0.42
1:G:89:ARG:NH1	1:G:111:ASP:OD1	2.46	0.42
1:A:153:ILE:O	1:A:157:GLU:HG2	2.20	0.42
1:B:168:LYS:HD2	1:B:198:ASP:HB2	2.01	0.42
1:C:133:LYS:HB2	1:C:133:LYS:NZ	2.35	0.42
1:E:13:MET:HE3	1:E:15:LEU:HD11	2.01	0.42
1:H:8:GLN:NE2	1:H:121:ILE:HD12	2.29	0.42
1:H:104:THR:O	1:H:278:GLY:HA2	2.20	0.42
1:A:92:ILE:HG22	1:A:93:MET:HE2	2.01	0.42
1:A:166:LEU:HD23	1:A:194:ARG:HB2	2.01	0.42
1:C:247:LEU:HD22	1:C:269:GLY:C	2.45	0.42
1:D:297:ALA:HB1	1:D:322:ILE:HD13	2.01	0.42
1:E:13:MET:CE	1:E:74:ASP:HA	2.48	0.42
1:F:131:GLY:HA2	1:H:89:ARG:HH21	1.85	0.42
1:H:43:ARG:HB2	1:H:53:PHE:CE1	2.54	0.42
1:D:13:MET:HE1	1:D:73:LEU:O	2.19	0.42
1:E:155:LEU:O	1:E:159:LEU:HG	2.20	0.42
1:G:56:ALA:O	1:G:58:PRO:HD3	2.20	0.42
1:A:185:LEU:C	1:A:185:LEU:HD23	2.44	0.42
1:D:173:PHE:CE1	1:D:174:ARG:HG3	2.55	0.42
1:B:226:PRO:HD2	1:B:235:MET:HE1	2.01	0.42
1:F:369:GLU:OE2	1:F:375:ARG:NE	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ILE:HG22	1:A:93:MET:CE	2.50	0.42
1:D:156:MET:HE2	1:D:190:PHE:CG	2.55	0.42
1:F:20:LEU:HA	1:F:21:PRO:HD3	1.87	0.42
1:F:227:VAL:HG12	1:F:231:HIS:CD2	2.55	0.42
1:F:156:MET:HE1	1:F:186:ILE:HG12	2.01	0.41
1:A:53:PHE:HB3	1:A:307:LEU:HD21	2.01	0.41
1:A:89:ARG:NH1	1:A:111:ASP:OD1	2.51	0.41
1:A:91:ALA:HB2	1:B:134:CYS:HA	2.01	0.41
1:D:13:MET:HG3	1:D:42:LEU:CD1	2.50	0.41
1:C:127:TRP:CZ2	1:C:133:LYS:HD2	2.55	0.41
1:B:133:LYS:HE2	1:B:136:ASP:OD1	2.20	0.41
1:D:89:ARG:CZ	1:D:115:LEU:HD21	2.50	0.41
1:D:364:ASP:HB3	1:D:367:LYS:HG3	2.02	0.41
1:F:104:THR:O	1:F:278:GLY:HA2	2.20	0.41
1:F:127:TRP:CH2	1:F:133:LYS:HD2	2.55	0.41
1:H:201:GLN:HB2	1:H:228:ARG:HA	2.02	0.41
1:A:116:ASP:O	1:A:120:ARG:HG2	2.20	0.41
1:C:275:MET:HB2	1:C:302:MET:CE	2.46	0.41
1:E:249:ASP:HB3	1:E:250:GLU:OE1	2.20	0.41
1:H:200:ASN:O	1:H:201:GLN:HG2	2.20	0.41
1:C:185:LEU:HD23	1:C:185:LEU:O	2.21	0.41
1:C:309:HIS:CG	1:C:328:PHE:HB3	2.56	0.41
1:E:59:TRP:HA	1:E:59:TRP:CE3	2.56	0.41
1:E:156:MET:HE1	1:E:186:ILE:HG23	2.03	0.41
1:F:73:LEU:HG	1:F:106:ALA:HB1	2.03	0.41
1:E:92:ILE:HG22	1:E:93:MET:CE	2.51	0.41
1:C:126:VAL:HB	1:C:314:HIS:CG	2.55	0.41
1:C:209:VAL:N	1:C:210:PRO:HD2	2.35	0.41
1:D:329:TYR:CD1	1:D:329:TYR:C	2.98	0.41
1:H:304:GLU:HG3	1:H:309:HIS:CD2	2.56	0.41
1:A:253:TYR:HA	1:A:276:LYS:HB3	2.03	0.41
1:B:127:TRP:CH2	1:B:133:LYS:HD2	2.56	0.41
1:C:166:LEU:HD23	1:C:194:ARG:HB2	2.03	0.41
1:D:104:THR:O	1:D:278:GLY:HA2	2.21	0.41
1:D:131:GLY:HA2	1:G:89:ARG:NH2	2.35	0.41
1:D:201:GLN:NE2	1:D:250:GLU:HG2	2.36	0.41
1:E:116:ASP:O	1:E:120:ARG:HG2	2.21	0.41
1:E:368:LEU:O	1:E:372:ALA:HB2	2.21	0.41
1:G:127:TRP:CE2	1:G:133:LYS:HD2	2.56	0.41
1:G:375:ARG:HG2	1:G:375:ARG:NH1	2.36	0.41
1:A:13:MET:HG3	1:A:42:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:H	1:A:192:GLU:CD	2.29	0.41
1:F:225:GLN:NE2	1:F:235:MET:CE	2.74	0.41
1:A:61:VAL:HG23	1:A:62:PHE:CD1	2.56	0.40
1:D:153:ILE:O	1:D:157:GLU:HG2	2.21	0.40
1:G:59:TRP:CD1	1:G:62:PHE:CD2	3.09	0.40
1:B:13:MET:HE3	1:B:15:LEU:CD1	2.48	0.40
1:C:249:ASP:HB3	1:C:250:GLU:OE1	2.22	0.40
1:D:280:LEU:N	1:D:280:LEU:HD12	2.36	0.40
1:E:182:ARG:O	1:E:186:ILE:HG13	2.21	0.40
1:A:302:MET:O	1:A:304:GLU:HG2	2.21	0.40
1:A:309:HIS:CE1	1:A:331:ALA:H	2.29	0.40
1:B:341:GLU:HG2	1:B:364:ASP:HB2	2.02	0.40
1:C:160:ARG:HD3	1:C:192:GLU:OE1	2.21	0.40
1:E:43:ARG:HG3	1:E:53:PHE:CZ	2.56	0.40
1:E:329:TYR:CD1	1:E:329:TYR:C	2.99	0.40
1:G:156:MET:CE	1:G:193:PHE:CE2	3.05	0.40
1:H:329:TYR:CD1	1:H:329:TYR:C	2.99	0.40
1:B:57:SER:OG	1:B:304:GLU:HB3	2.21	0.40
1:F:63:THR:HG21	1:F:302:MET:CE	2.43	0.40
1:F:253:TYR:HA	1:F:276:LYS:HB3	2.04	0.40
1:H:149:PHE:HE2	1:H:185:LEU:HD13	1.87	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	352/385 (91%)	343 (97%)	9 (3%)	0	100	100
1	B	352/385 (91%)	341 (97%)	11 (3%)	0	100	100
1	C	352/385 (91%)	341 (97%)	11 (3%)	0	100	100
1	D	352/385 (91%)	339 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	352/385 (91%)	342 (97%)	10 (3%)	0	100	100
1	F	352/385 (91%)	342 (97%)	10 (3%)	0	100	100
1	G	352/385 (91%)	343 (97%)	9 (3%)	0	100	100
1	H	352/385 (91%)	341 (97%)	11 (3%)	0	100	100
All	All	2816/3080 (91%)	2732 (97%)	84 (3%)	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	277/299 (93%)	274 (99%)	3 (1%)	65	54
1	B	277/299 (93%)	271 (98%)	6 (2%)	45	29
1	C	277/299 (93%)	274 (99%)	3 (1%)	65	54
1	D	277/299 (93%)	272 (98%)	5 (2%)	51	36
1	E	277/299 (93%)	275 (99%)	2 (1%)	76	69
1	F	277/299 (93%)	273 (99%)	4 (1%)	59	46
1	G	277/299 (93%)	274 (99%)	3 (1%)	65	54
1	H	277/299 (93%)	276 (100%)	1 (0%)	84	80
All	All	2216/2392 (93%)	2189 (99%)	27 (1%)	63	51

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	MET
1	A	247	LEU
1	A	315	MET
1	B	130	LEU
1	B	181	MET
1	B	214	ASP

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Mol	Chain	Res	Type
1	B	246	LEU
1	B	301	ASP
1	B	304	GLU
1	C	133	LYS
1	C	181	MET
1	C	304	GLU
1	D	181	MET
1	D	214	ASP
1	D	301	ASP
1	D	304	GLU
1	D	315	MET
1	E	181	MET
1	E	214	ASP
1	F	181	MET
1	F	235	MET
1	F	258	MET
1	F	301	ASP
1	G	129	LEU
1	G	181	MET
1	G	214	ASP
1	H	214	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	HIS
1	A	350	GLN
1	B	284	GLN
1	B	309	HIS
1	B	350	GLN
1	C	8	GLN
1	C	200	ASN
1	C	263	HIS
1	C	309	HIS
1	C	370	HIS
1	D	8	GLN
1	D	102	HIS
1	D	123	ASN
1	D	200	ASN
1	D	309	HIS
1	D	350	GLN
1	E	102	HIS

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Mol	Chain	Res	Type
1	E	200	ASN
1	E	284	GLN
1	E	309	HIS
1	F	8	GLN
1	F	102	HIS
1	F	200	ASN
1	F	231	HIS
1	F	263	HIS
1	F	309	HIS
1	F	336	ASN
1	F	350	GLN
1	G	8	GLN
1	G	200	ASN
1	G	284	GLN
1	G	309	HIS
1	G	350	GLN
1	H	102	HIS
1	H	200	ASN
1	H	309	HIS
1	H	350	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	356/385 (92%)	0.53	13 (3%)	45	49	20, 31, 44, 54	0
1	B	356/385 (92%)	0.59	18 (5%)	33	37	21, 31, 46, 67	0
1	C	356/385 (92%)	0.71	16 (4%)	38	42	23, 34, 46, 59	0
1	D	356/385 (92%)	0.74	28 (7%)	18	20	21, 32, 50, 61	0
1	E	356/385 (92%)	0.82	44 (12%)	8	8	21, 34, 49, 57	0
1	F	356/385 (92%)	0.56	18 (5%)	33	37	21, 32, 44, 56	0
1	G	356/385 (92%)	0.24	12 (3%)	48	52	19, 27, 41, 52	0
1	H	356/385 (92%)	0.93	42 (11%)	9	9	22, 35, 55, 65	0
All	All	2848/3080 (92%)	0.64	191 (6%)	24	26	19, 32, 48, 67	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	PHE	6.0
1	H	6	LEU	5.5
1	C	62	PHE	5.4
1	F	235	MET	5.0
1	E	62	PHE	4.8
1	D	22	VAL	4.5
1	H	121	ILE	4.4
1	H	62	PHE	4.4
1	B	62	PHE	4.1
1	G	62	PHE	4.0
1	F	62	PHE	3.9
1	B	375	ARG	3.9
1	D	16	TRP	3.6
1	D	121	ILE	3.6
1	E	178	PHE	3.6
1	H	375	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	62	PHE	3.5
1	H	372	ALA	3.5
1	H	16	TRP	3.5
1	E	375	ARG	3.5
1	E	22	VAL	3.5
1	B	373	VAL	3.4
1	H	373	VAL	3.4
1	E	153	ILE	3.4
1	C	375	ARG	3.3
1	D	59	TRP	3.3
1	E	61	VAL	3.3
1	E	59	TRP	3.2
1	H	11	ILE	3.2
1	E	19	ALA	3.2
1	H	53	PHE	3.2
1	H	145	ALA	3.2
1	C	6	LEU	3.1
1	H	8	GLN	3.1
1	E	189	ASP	3.1
1	D	46	ALA	3.1
1	H	22	VAL	3.1
1	H	80	LEU	3.1
1	H	368	LEU	3.1
1	A	22	VAL	3.0
1	E	180	ILE	3.0
1	D	372	ALA	3.0
1	C	80	LEU	3.0
1	D	375	ARG	3.0
1	H	366	GLU	3.0
1	D	363	ALA	3.0
1	E	151	ALA	3.0
1	H	334	PHE	3.0
1	D	373	VAL	2.9
1	C	59	TRP	2.9
1	H	59	TRP	2.9
1	E	190	PHE	2.9
1	E	80	LEU	2.9
1	F	6	LEU	2.8
1	F	375	ARG	2.8
1	D	50	ALA	2.8
1	E	158	ARG	2.8
1	B	121	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	49	GLY	2.8
1	E	193	PHE	2.7
1	E	147	PRO	2.7
1	B	80	LEU	2.7
1	B	372	ALA	2.7
1	G	59	TRP	2.7
1	C	241	LEU	2.7
1	H	86	VAL	2.7
1	H	371	TYR	2.7
1	G	121	ILE	2.7
1	D	345	ARG	2.6
1	H	369	GLU	2.6
1	A	334	PHE	2.6
1	F	361	ALA	2.6
1	C	90	VAL	2.6
1	E	121	ILE	2.6
1	H	151	ALA	2.6
1	E	191	PRO	2.6
1	F	85	ARG	2.6
1	E	185	LEU	2.6
1	E	368	LEU	2.6
1	E	161	ALA	2.6
1	E	342	THR	2.5
1	H	150	ASP	2.5
1	E	173	PHE	2.5
1	B	6	LEU	2.5
1	A	59	TRP	2.5
1	E	16	TRP	2.5
1	D	43	ARG	2.5
1	A	80	LEU	2.5
1	F	343	PRO	2.5
1	C	342	THR	2.5
1	F	188	ARG	2.5
1	D	368	LEU	2.4
1	H	77	LEU	2.4
1	D	365	PRO	2.4
1	G	48	GLY	2.4
1	G	375	ARG	2.4
1	E	348	ALA	2.4
1	F	121	ILE	2.4
1	A	7	GLU	2.4
1	H	365	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	334	PHE	2.4
1	G	336	ASN	2.4
1	D	322	ILE	2.4
1	H	10	ILE	2.4
1	E	148	ASP	2.4
1	G	80	LEU	2.4
1	B	16	TRP	2.4
1	E	303	PHE	2.4
1	C	369	GLU	2.4
1	H	367	LYS	2.4
1	F	22	VAL	2.4
1	B	336	ASN	2.3
1	A	161	ALA	2.3
1	D	80	LEU	2.3
1	D	307	LEU	2.3
1	E	6	LEU	2.3
1	E	20	LEU	2.3
1	E	154	ALA	2.3
1	E	149	PHE	2.3
1	A	375	ARG	2.3
1	F	372	ALA	2.3
1	D	371	TYR	2.3
1	C	373	VAL	2.3
1	G	22	VAL	2.3
1	B	59	TRP	2.2
1	E	365	PRO	2.2
1	F	366	GLU	2.2
1	E	37	CYS	2.2
1	H	12	ALA	2.2
1	B	362	ARG	2.2
1	F	158	ARG	2.2
1	D	241	LEU	2.2
1	G	6	LEU	2.2
1	B	22	VAL	2.2
1	G	45	VAL	2.2
1	D	343	PRO	2.2
1	B	151	ALA	2.2
1	C	151	ALA	2.2
1	H	361	ALA	2.2
1	E	155	LEU	2.2
1	H	20	LEU	2.2
1	G	47	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	303	PHE	2.2
1	A	153	ILE	2.2
1	C	352	ILE	2.2
1	H	82	ILE	2.2
1	D	336	ASN	2.2
1	F	342	THR	2.2
1	C	22	VAL	2.2
1	E	372	ALA	2.2
1	H	19	ALA	2.2
1	H	340	LEU	2.2
1	F	43	ARG	2.2
1	C	173	PHE	2.2
1	H	173	PHE	2.2
1	H	303	PHE	2.2
1	A	121	ILE	2.2
1	H	7	GLU	2.1
1	H	46	ALA	2.1
1	E	144	ILE	2.1
1	E	186	ILE	2.1
1	E	174	ARG	2.1
1	B	161	ALA	2.1
1	E	361	ALA	2.1
1	F	151	ALA	2.1
1	F	373	VAL	2.1
1	H	351	VAL	2.1
1	H	363	ALA	2.1
1	B	340	LEU	2.1
1	A	366	GLU	2.1
1	B	367	LYS	2.1
1	D	361	ALA	2.1
1	H	90	VAL	2.1
1	C	303	PHE	2.1
1	E	253	TYR	2.1
1	B	7	GLU	2.0
1	B	145	ALA	2.0
1	C	372	ALA	2.0
1	D	6	LEU	2.0
1	H	18	LEU	2.0
1	D	342	THR	2.0
1	G	342	THR	2.0
1	E	21	PRO	2.0
1	D	49	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	158	ARG	2.0
1	H	193	PHE	2.0
1	A	214	ASP	2.0
1	A	346	VAL	2.0
1	E	373	VAL	2.0
1	F	346	VAL	2.0
1	E	370	HIS	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(Å ²)	Q<0.9
2	MG	H	386	1/1	0.88	0.11	39,39,39,39	0
2	MG	B	386	1/1	0.89	0.09	36,36,36,36	0
2	MG	E	386	1/1	0.95	0.12	36,36,36,36	0
2	MG	F	386	1/1	0.95	0.10	33,33,33,33	0
2	MG	C	386	1/1	0.95	0.07	40,40,40,40	0
2	MG	G	386	1/1	0.96	0.06	30,30,30,30	0
3	NA	D	387	1/1	0.96	0.05	31,31,31,31	0
3	NA	H	387	1/1	0.96	0.08	28,28,28,28	0
3	NA	C	387	1/1	0.97	0.06	31,31,31,31	0
2	MG	A	386	1/1	0.97	0.08	36,36,36,36	0
3	NA	E	387	1/1	0.97	0.04	27,27,27,27	0
2	MG	D	386	1/1	0.97	0.07	37,37,37,37	0
3	NA	A	387	1/1	0.98	0.04	28,28,28,28	0
3	NA	F	387	1/1	0.98	0.04	26,26,26,26	0
3	NA	G	387	1/1	0.98	0.04	23,23,23,23	0
3	NA	B	387	1/1	0.98	0.04	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.