



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:03 AM UTC

PDB ID : 3I4K / pdb_00003i4k
Title : Crystal structure of Muconate lactonizing enzyme from *Corynebacterium glutamicum*
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 : 2009-07-01
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

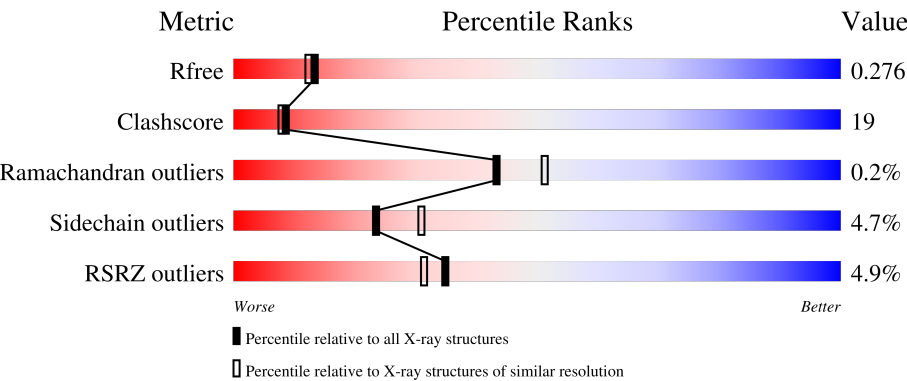
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	383	3% 66% 27% ..
1	B	383	2% 65% 29% ...
1	C	383	3% 61% 31% ..
1	D	383	7% 66% 27% ..
1	E	383	2% 69% 24% ..

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Mol	Chain	Length	Quality of chain
1	F	383	5% 67% 27%
1	G	383	9% 60% 35%
1	H	383	7% 62% 31%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23024 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 lactonizing enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	B	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	C	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	D	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	E	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	F	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	G	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	H	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q8NN12
A	2	SER	-	expression tag	UNP Q8NN12
A	3	LEU	-	expression tag	UNP Q8NN12
A	376	GLU	-	expression tag	UNP Q8NN12
A	377	GLY	-	expression tag	UNP Q8NN12
A	378	HIS	-	expression tag	UNP Q8NN12
A	379	HIS	-	expression tag	UNP Q8NN12
A	380	HIS	-	expression tag	UNP Q8NN12
A	381	HIS	-	expression tag	UNP Q8NN12
A	382	HIS	-	expression tag	UNP Q8NN12
A	383	HIS	-	expression tag	UNP Q8NN12
B	1	MSE	-	expression tag	UNP Q8NN12
B	2	SER	-	expression tag	UNP Q8NN12

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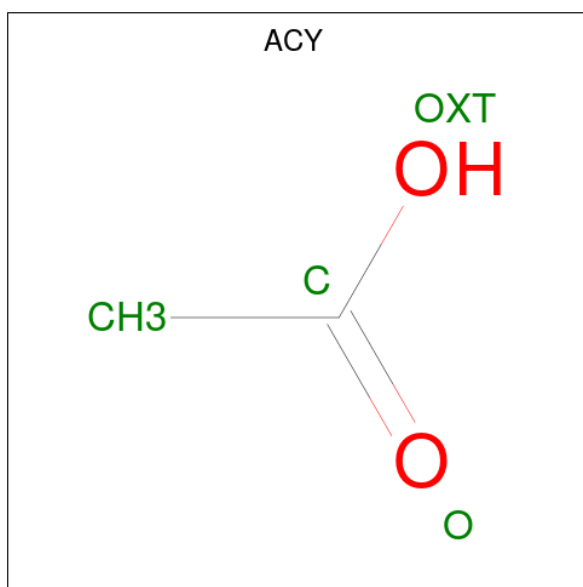
Chain	Residue	Modelled	Actual	Comment	Reference
B	3	LEU	-	expression tag	UNP Q8NN12
B	376	GLU	-	expression tag	UNP Q8NN12
B	377	GLY	-	expression tag	UNP Q8NN12
B	378	HIS	-	expression tag	UNP Q8NN12
B	379	HIS	-	expression tag	UNP Q8NN12
B	380	HIS	-	expression tag	UNP Q8NN12
B	381	HIS	-	expression tag	UNP Q8NN12
B	382	HIS	-	expression tag	UNP Q8NN12
B	383	HIS	-	expression tag	UNP Q8NN12
C	1	MSE	-	expression tag	UNP Q8NN12
C	2	SER	-	expression tag	UNP Q8NN12
C	3	LEU	-	expression tag	UNP Q8NN12
C	376	GLU	-	expression tag	UNP Q8NN12
C	377	GLY	-	expression tag	UNP Q8NN12
C	378	HIS	-	expression tag	UNP Q8NN12
C	379	HIS	-	expression tag	UNP Q8NN12
C	380	HIS	-	expression tag	UNP Q8NN12
C	381	HIS	-	expression tag	UNP Q8NN12
C	382	HIS	-	expression tag	UNP Q8NN12
C	383	HIS	-	expression tag	UNP Q8NN12
D	1	MSE	-	expression tag	UNP Q8NN12
D	2	SER	-	expression tag	UNP Q8NN12
D	3	LEU	-	expression tag	UNP Q8NN12
D	376	GLU	-	expression tag	UNP Q8NN12
D	377	GLY	-	expression tag	UNP Q8NN12
D	378	HIS	-	expression tag	UNP Q8NN12
D	379	HIS	-	expression tag	UNP Q8NN12
D	380	HIS	-	expression tag	UNP Q8NN12
D	381	HIS	-	expression tag	UNP Q8NN12
D	382	HIS	-	expression tag	UNP Q8NN12
D	383	HIS	-	expression tag	UNP Q8NN12
E	1	MSE	-	expression tag	UNP Q8NN12
E	2	SER	-	expression tag	UNP Q8NN12
E	3	LEU	-	expression tag	UNP Q8NN12
E	376	GLU	-	expression tag	UNP Q8NN12
E	377	GLY	-	expression tag	UNP Q8NN12
E	378	HIS	-	expression tag	UNP Q8NN12
E	379	HIS	-	expression tag	UNP Q8NN12
E	380	HIS	-	expression tag	UNP Q8NN12
E	381	HIS	-	expression tag	UNP Q8NN12
E	382	HIS	-	expression tag	UNP Q8NN12
E	383	HIS	-	expression tag	UNP Q8NN12

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MSE	-	expression tag	UNP Q8NN12
F	2	SER	-	expression tag	UNP Q8NN12
F	3	LEU	-	expression tag	UNP Q8NN12
F	376	GLU	-	expression tag	UNP Q8NN12
F	377	GLY	-	expression tag	UNP Q8NN12
F	378	HIS	-	expression tag	UNP Q8NN12
F	379	HIS	-	expression tag	UNP Q8NN12
F	380	HIS	-	expression tag	UNP Q8NN12
F	381	HIS	-	expression tag	UNP Q8NN12
F	382	HIS	-	expression tag	UNP Q8NN12
F	383	HIS	-	expression tag	UNP Q8NN12
G	1	MSE	-	expression tag	UNP Q8NN12
G	2	SER	-	expression tag	UNP Q8NN12
G	3	LEU	-	expression tag	UNP Q8NN12
G	376	GLU	-	expression tag	UNP Q8NN12
G	377	GLY	-	expression tag	UNP Q8NN12
G	378	HIS	-	expression tag	UNP Q8NN12
G	379	HIS	-	expression tag	UNP Q8NN12
G	380	HIS	-	expression tag	UNP Q8NN12
G	381	HIS	-	expression tag	UNP Q8NN12
G	382	HIS	-	expression tag	UNP Q8NN12
G	383	HIS	-	expression tag	UNP Q8NN12
H	1	MSE	-	expression tag	UNP Q8NN12
H	2	SER	-	expression tag	UNP Q8NN12
H	3	LEU	-	expression tag	UNP Q8NN12
H	376	GLU	-	expression tag	UNP Q8NN12
H	377	GLY	-	expression tag	UNP Q8NN12
H	378	HIS	-	expression tag	UNP Q8NN12
H	379	HIS	-	expression tag	UNP Q8NN12
H	380	HIS	-	expression tag	UNP Q8NN12
H	381	HIS	-	expression tag	UNP Q8NN12
H	382	HIS	-	expression tag	UNP Q8NN12
H	383	HIS	-	expression tag	UNP Q8NN12

- Molecule 2 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

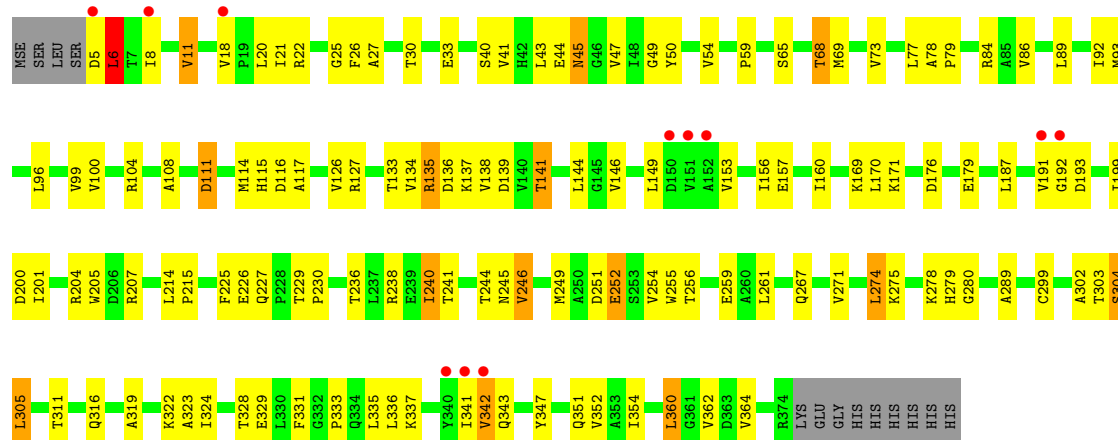
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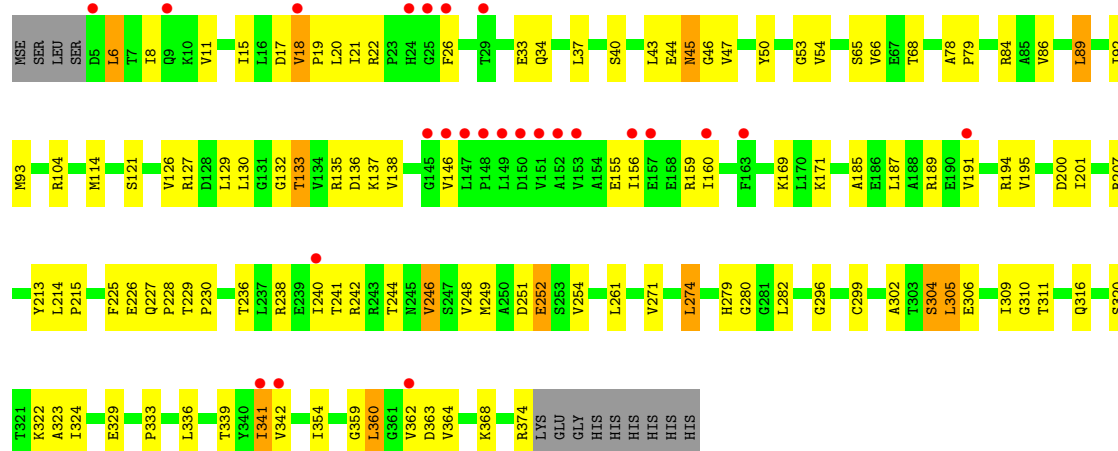
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

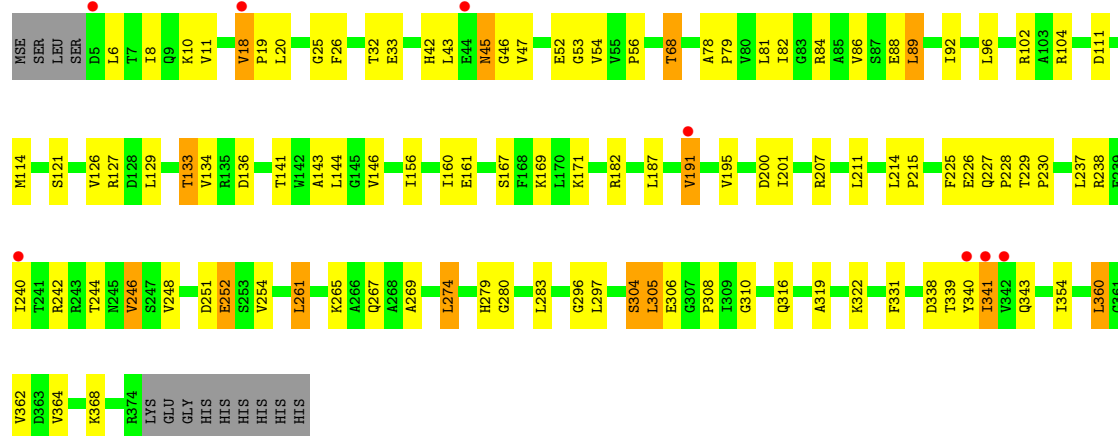
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total 73	O 73	0	0
4	B	75	Total 75	O 75	0	0
4	C	56	Total 56	O 56	0	0
4	D	72	Total 72	O 72	0	0
4	E	98	Total 98	O 98	0	0
4	F	65	Total 65	O 65	0	0
4	G	28	Total 28	O 28	0	0
4	H	45	Total 45	O 45	0	0



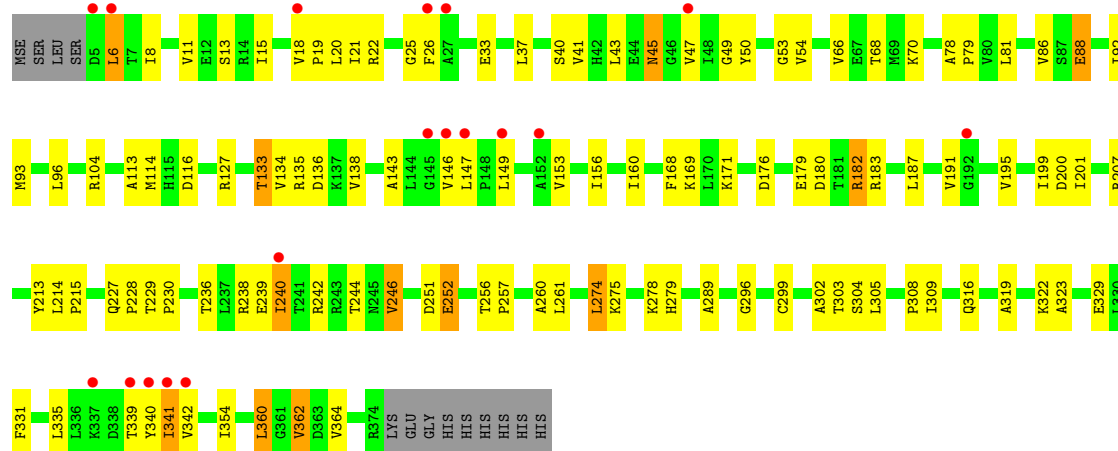
• Molecule 1: Muconate lactonizing enzyme



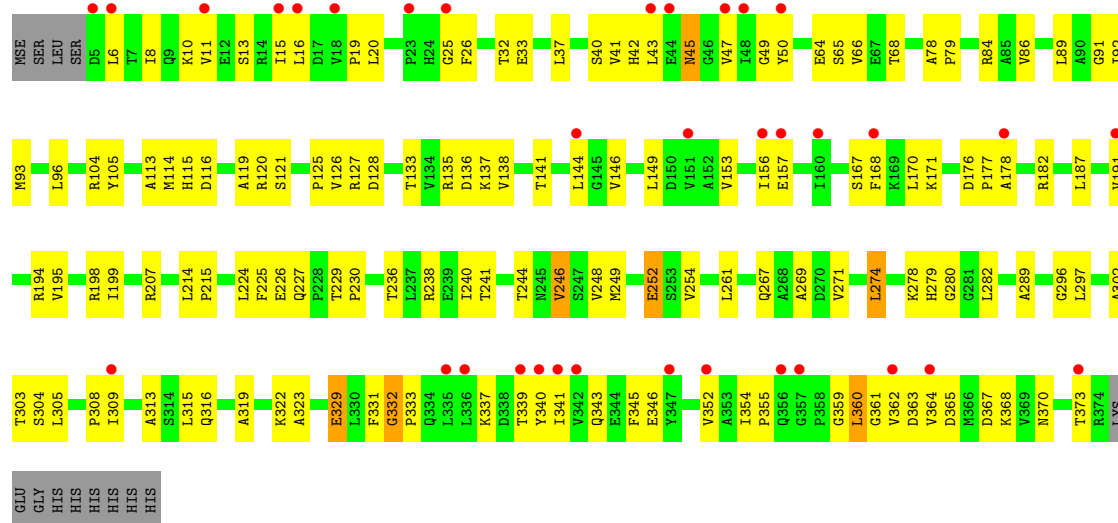
• Molecule 1: Muconate lactonizing enzyme



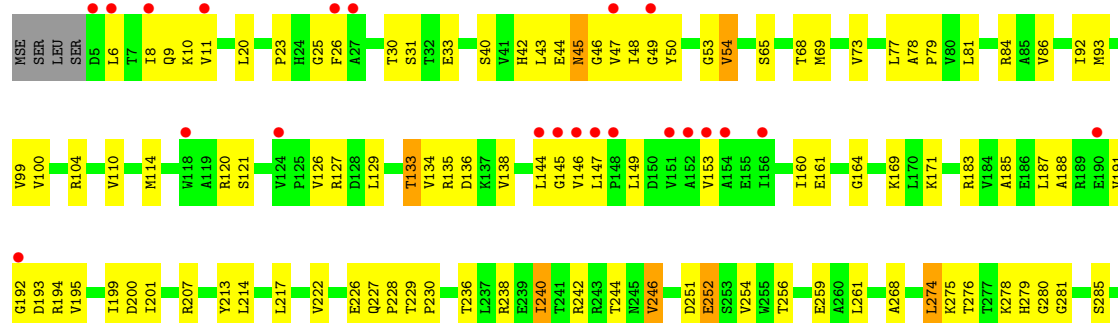
• Molecule 1: Muconate lactonizing enzyme



• Molecule 1: Muconate lactonizing enzyme



• Molecule 1: Muconate lactonizing enzyme





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.54Å 156.71Å 202.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.92 – 2.20 24.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.92-2.20) 99.6 (24.92-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.277 0.244 , 0.276	Depositor DCC
R_{free} test set	11688 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23024	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: MG, ACY

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	0/2853	0.96	14/3871 (0.4%)
1	B	0.43	0/2853	0.97	11/3871 (0.3%)
1	C	0.40	0/2853	0.94	7/3871 (0.2%)
1	D	0.41	0/2853	0.95	8/3871 (0.2%)
1	E	0.43	0/2853	0.98	11/3871 (0.3%)
1	F	0.41	0/2853	0.94	7/3871 (0.2%)
1	G	0.39	0/2853	0.92	4/3871 (0.1%)
1	H	0.41	0/2853	0.96	11/3871 (0.3%)
All	All	0.41	0/22824	0.95	73/30968 (0.2%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	341	ILE	N-CA-C	8.45	120.84	111.88
1	A	304	SER	N-CA-C	-8.01	103.59	112.72
1	E	134	VAL	N-CA-C	-7.96	105.00	112.96
1	D	304	SER	N-CA-C	-7.62	104.03	112.72
1	F	304	SER	N-CA-C	-7.57	104.10	112.72
1	E	304	SER	N-CA-C	-7.49	104.19	112.72
1	H	304	SER	N-CA-C	-7.16	103.86	112.59
1	C	54	VAL	N-CA-C	7.08	117.70	108.35
1	B	304	SER	N-CA-C	-6.97	104.08	112.59
1	C	304	SER	N-CA-C	-6.96	104.78	112.72
1	B	6	LEU	N-CA-C	-6.88	104.51	113.17
1	D	254	VAL	N-CA-C	6.75	118.02	107.28
1	H	341	ILE	N-CA-C	6.69	119.59	113.10
1	A	32	THR	N-CA-C	-6.53	105.05	114.12
1	G	304	SER	N-CA-C	-6.45	103.75	112.26
1	E	54	VAL	N-CA-C	6.42	117.96	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	32	THR	N-CA-C	-6.39	105.64	113.50
1	G	254	VAL	N-CA-C	6.39	117.97	107.24
1	A	54	VAL	N-CA-C	6.21	116.55	108.35
1	A	324	ILE	N-CA-C	-6.17	96.52	109.34
1	B	82	ILE	N-CA-C	6.15	117.23	108.93
1	D	341	ILE	N-CA-C	6.12	118.06	112.43
1	A	134	VAL	N-CA-C	-6.01	106.94	112.96
1	H	213	TYR	N-CA-C	6.01	119.09	111.69
1	B	32	THR	N-CA-C	-6.00	106.30	113.97
1	F	88	GLU	N-CA-C	-5.98	105.29	112.59
1	B	341	ILE	N-CA-C	5.85	121.51	109.34
1	H	53	GLY	N-CA-C	-5.82	99.38	113.18
1	D	129	LEU	N-CA-C	-5.81	106.24	113.38
1	E	82	ILE	N-CA-C	5.78	116.73	108.93
1	E	254	VAL	N-CA-C	5.74	115.85	106.72
1	B	195	VAL	N-CA-C	5.73	117.16	108.80
1	A	129	LEU	N-CA-C	-5.71	105.97	113.17
1	D	213	TYR	N-CA-C	5.63	120.28	112.90
1	H	254	VAL	N-CA-C	5.63	116.63	106.61
1	C	134	VAL	N-CA-C	-5.59	106.88	113.42
1	A	75	GLY	N-CA-C	5.56	121.55	114.66
1	H	281	GLY	N-CA-C	5.49	117.67	111.85
1	H	54	VAL	N-CA-C	5.47	115.56	108.35
1	H	194	ARG	N-CA-C	5.44	118.13	111.82
1	H	268	ALA	N-CA-C	5.43	119.76	113.18
1	F	213	TYR	N-CA-C	5.42	119.99	112.45
1	D	194	ARG	N-CA-C	5.42	118.02	111.40
1	C	324	ILE	N-CA-C	-5.41	98.09	109.34
1	E	129	LEU	N-CA-C	-5.41	106.36	113.17
1	E	53	GLY	N-CA-C	-5.40	100.38	113.18
1	A	341	ILE	N-CA-C	5.40	117.40	112.43
1	B	254	VAL	N-CA-C	5.39	116.21	106.61
1	E	88	GLU	N-CA-C	-5.39	106.57	112.72
1	F	6	LEU	N-CA-C	-5.38	106.49	113.16
1	E	32	THR	N-CA-C	-5.38	107.09	113.97
1	A	254	VAL	N-CA-C	5.36	116.15	106.61
1	B	129	LEU	N-CA-C	-5.35	106.42	113.17
1	B	53	GLY	N-CA-C	-5.33	100.55	113.18
1	A	281	GLY	N-CA-C	5.31	117.45	112.08
1	H	329	GLU	N-CA-C	-5.31	104.60	111.71
1	H	129	LEU	N-CA-C	-5.30	106.86	113.38
1	G	329	GLU	N-CA-C	-5.25	104.67	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	VAL	N-CA-C	5.24	116.04	107.24
1	F	53	GLY	N-CA-C	-5.21	100.82	113.18
1	A	53	GLY	N-CA-C	-5.17	100.93	113.18
1	C	255	TRP	N-CA-C	-5.17	106.92	113.43
1	B	281	GLY	N-CA-C	5.16	117.29	112.08
1	A	52	GLU	N-CA-C	5.16	117.38	109.07
1	E	191	VAL	N-CA-C	5.16	116.08	111.90
1	A	329	GLU	N-CA-C	-5.12	104.21	110.61
1	F	260	ALA	N-CA-C	-5.12	105.78	111.36
1	D	53	GLY	N-CA-C	-5.11	101.07	113.18
1	F	134	VAL	N-CA-C	-5.08	107.88	112.96
1	D	324	ILE	N-CA-C	-5.06	98.81	109.34
1	B	134	VAL	N-CA-C	-5.05	107.91	112.96
1	A	6	LEU	N-CA-C	-5.03	106.98	113.02
1	C	6	LEU	N-CA-C	-5.02	107.00	113.02

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	2809	0	2829	105	0
1	B	2809	0	2829	114	0
1	C	2809	0	2829	110	0
1	D	2809	0	2829	102	0
1	E	2809	0	2829	98	0
1	F	2809	0	2829	101	0
1	G	2809	0	2829	127	0
1	H	2809	0	2829	112	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	4	0	3	0	0
2	H	4	0	3	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	73	0	0	2	0
4	B	75	0	0	4	0
4	C	56	0	0	0	0
4	D	72	0	0	3	0
4	E	98	0	0	4	0
4	F	65	0	0	1	0
4	G	28	0	0	0	0
4	H	45	0	0	2	0
All	All	23024	0	22656	855	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 19.

All (855) 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:H:45:ASN:HD21	1:H:47:VAL:HG12	1.05	1.17
1:D:45:ASN:HD21	1:D:47:VAL:HG12	1.04	1.13
1:E:45:ASN:HD21	1:E:47:VAL:HG12	1.02	1.11
1:C:45:ASN:HD21	1:C:47:VAL:HG12	1.09	1.08
1:H:227:GLN:HG2	1:H:252:GLU:HG2	1.35	1.05
1:G:227:GLN:HG2	1:G:252:GLU:HG2	1.42	1.02
1:B:227:GLN:HG2	1:B:252:GLU:HG2	1.43	1.01
1:A:227:GLN:HG2	1:A:252:GLU:HG2	1.39	1.00
1:C:227:GLN:HG2	1:C:252:GLU:HG2	1.42	0.99
1:F:45:ASN:HD21	1:F:47:VAL:HG12	1.27	0.99
1:F:227:GLN:HG2	1:F:252:GLU:HG2	1.45	0.99
1:C:45:ASN:ND2	1:C:47:VAL:HG12	1.80	0.97
1:E:227:GLN:HG2	1:E:252:GLU:HG2	1.45	0.96
1:D:227:GLN:HG2	1:D:252:GLU:HG2	1.49	0.94
1:E:68:THR:HG22	4:E:452:HOH:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASN:HD21	1:B:47:VAL:HG12	1.33	0.92
1:C:92:ILE:HD12	1:C:114:MSE:HE1	1.51	0.92
1:A:45:ASN:ND2	1:A:47:VAL:HG12	1.85	0.92
1:E:45:ASN:ND2	1:E:47:VAL:HG12	1.85	0.90
1:A:15:ILE:HG23	1:A:66:VAL:HG21	1.54	0.89
1:D:45:ASN:ND2	1:D:47:VAL:HG12	1.88	0.87
1:G:45:ASN:HD21	1:G:47:VAL:HG12	1.40	0.86
1:A:45:ASN:HD21	1:A:47:VAL:HG12	1.40	0.86
1:G:141:THR:HG22	1:G:167:SER:OG	1.75	0.85
1:A:11:VAL:HG21	1:A:78:ALA:HB1	1.57	0.85
1:H:126:VAL:HG21	1:H:360:LEU:HD12	1.60	0.84
1:B:45:ASN:ND2	1:B:47:VAL:HG12	1.93	0.83
1:H:45:ASN:ND2	1:H:47:VAL:HG12	1.90	0.83
1:B:11:VAL:HG21	1:B:78:ALA:HB1	1.61	0.82
1:D:68:THR:HG22	4:D:390:HOH:O	1.80	0.82
1:G:227:GLN:HG2	1:G:252:GLU:CG	2.11	0.81
1:G:156:ILE:HG21	1:G:191:VAL:HG11	1.63	0.80
1:F:20:LEU:HD13	1:F:33:GLU:HA	1.62	0.80
1:E:92:ILE:HD13	1:E:114:MSE:HE1	1.62	0.80
1:B:141:THR:HG22	1:B:167:SER:OG	1.82	0.79
1:F:92:ILE:HD13	1:F:114:MSE:HE1	1.64	0.79
1:D:15:ILE:HG23	1:D:66:VAL:HG21	1.64	0.78
1:F:93:MSE:HA	1:F:93:MSE:HE2	1.65	0.77
1:E:43:LEU:HD12	1:E:47:VAL:CG1	2.14	0.77
1:D:86:VAL:HG23	1:D:114:MSE:HE2	1.66	0.77
1:B:11:VAL:CG2	1:B:78:ALA:HB1	2.15	0.77
1:B:20:LEU:HD13	1:B:33:GLU:HA	1.67	0.76
1:A:11:VAL:CG2	1:A:78:ALA:HB1	2.15	0.76
1:F:227:GLN:HG2	1:F:252:GLU:CG	2.15	0.76
1:E:227:GLN:HG2	1:E:252:GLU:CG	2.16	0.76
1:G:45:ASN:ND2	1:G:47:VAL:HG12	2.00	0.76
1:B:127:ARG:HD2	1:B:133:THR:HG22	1.66	0.76
1:A:227:GLN:HG2	1:A:252:GLU:CG	2.14	0.75
1:E:45:ASN:HD21	1:E:47:VAL:CG1	1.91	0.75
1:E:127:ARG:HD2	1:E:133:THR:HG22	1.68	0.75
1:C:135:ARG:HD2	1:C:138:VAL:HG12	1.67	0.75
1:F:15:ILE:HG23	1:F:66:VAL:HG21	1.69	0.74
1:C:135:ARG:HH11	1:C:135:ARG:HB3	1.53	0.74
1:B:341:ILE:HD12	1:B:364:VAL:HA	1.70	0.73
1:H:227:GLN:HG2	1:H:252:GLU:CG	2.15	0.73
1:E:20:LEU:HD13	1:E:33:GLU:HA	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:GLN:HG2	1:D:252:GLU:CG	2.19	0.72
1:H:127:ARG:HH11	1:H:316:GLN:HE22	1.36	0.72
1:D:6:LEU:O	1:D:43:LEU:HD22	1.90	0.71
1:G:15:ILE:HG23	1:G:66:VAL:HG21	1.72	0.71
1:B:6:LEU:HG	1:B:86:VAL:HG12	1.72	0.71
1:C:20:LEU:HD13	1:C:33:GLU:HA	1.73	0.71
1:C:236:THR:O	1:C:240:ILE:HG23	1.89	0.71
1:D:11:VAL:HG21	1:D:78:ALA:HB1	1.71	0.71
1:B:227:GLN:HG2	1:B:252:GLU:CG	2.21	0.71
1:G:341:ILE:HG13	1:G:362:VAL:HG22	1.70	0.70
1:E:81:LEU:HD23	1:E:114:MSE:HE3	1.73	0.70
1:B:43:LEU:HB2	1:B:45:ASN:HD21	1.55	0.70
1:E:11:VAL:CG2	1:E:78:ALA:HB1	2.21	0.70
1:G:319:ALA:HB2	1:G:354:ILE:HG12	1.72	0.70
1:A:341:ILE:HG13	1:A:362:VAL:HG22	1.72	0.69
1:D:240:ILE:HD11	1:D:248:VAL:HG22	1.72	0.69
1:E:11:VAL:HG21	1:E:78:ALA:HB1	1.73	0.69
1:B:93:MSE:HE2	1:B:93:MSE:HA	1.73	0.69
1:B:341:ILE:HG13	1:B:362:VAL:HG22	1.74	0.69
1:G:240:ILE:HD11	1:G:248:VAL:HG22	1.74	0.69
1:A:20:LEU:HD13	1:A:33:GLU:HA	1.74	0.69
1:B:156:ILE:HG21	1:B:191:VAL:HG11	1.75	0.69
1:G:135:ARG:HD2	1:G:138:VAL:HG12	1.74	0.69
1:B:68:THR:HG22	4:B:430:HOH:O	1.93	0.68
1:B:156:ILE:O	1:B:160:ILE:HG13	1.92	0.68
1:B:339:THR:O	1:B:368:LYS:HD3	1.93	0.68
1:C:156:ILE:O	1:C:160:ILE:HG13	1.93	0.68
1:C:341:ILE:HD12	1:C:364:VAL:HA	1.75	0.68
1:C:227:GLN:HG2	1:C:252:GLU:CG	2.20	0.68
1:D:20:LEU:HD13	1:D:33:GLU:HA	1.76	0.67
1:H:6:LEU:HG	1:H:86:VAL:HG12	1.76	0.67
1:E:171:LYS:HE3	4:E:407:HOH:O	1.94	0.67
1:H:45:ASN:C	1:H:45:ASN:HD22	2.01	0.67
1:D:11:VAL:CG2	1:D:78:ALA:HB1	2.24	0.67
1:B:214:LEU:HD13	1:B:240:ILE:HD12	1.77	0.67
1:G:41:VAL:HG23	1:G:113:ALA:HB1	1.77	0.67
1:F:341:ILE:HD12	1:F:364:VAL:HA	1.77	0.67
1:G:127:ARG:H	1:G:316:GLN:HE21	1.42	0.66
1:H:149:LEU:O	1:H:153:VAL:HG23	1.94	0.66
1:H:68:THR:HG22	4:H:403:HOH:O	1.94	0.66
1:E:45:ASN:C	1:E:45:ASN:HD22	2.02	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:ILE:HG13	1:D:362:VAL:HG22	1.77	0.66
1:E:26:PHE:CE1	1:E:171:LYS:HE2	2.31	0.66
1:A:136:ASP:C	1:A:354:ILE:HD13	2.21	0.66
1:H:127:ARG:HB3	1:H:316:GLN:HE21	1.59	0.66
1:H:126:VAL:HG23	1:H:359:GLY:C	2.21	0.66
1:D:136:ASP:C	1:D:354:ILE:HD13	2.21	0.65
1:H:11:VAL:HG21	1:H:78:ALA:HB1	1.78	0.65
1:G:10:LYS:HE3	1:G:42:HIS:CD2	2.31	0.65
1:E:339:THR:O	1:E:368:LYS:HD3	1.96	0.65
1:E:341:ILE:HD12	1:E:364:VAL:HA	1.79	0.65
1:G:127:ARG:H	1:G:316:GLN:NE2	1.94	0.65
1:H:8:ILE:HD11	1:H:86:VAL:HB	1.77	0.65
1:A:274:LEU:HD13	1:A:279:HIS:CD2	2.31	0.65
1:G:302:ALA:HA	1:G:329:GLU:HG2	1.79	0.65
1:D:236:THR:O	1:D:240:ILE:HG23	1.96	0.65
1:F:227:GLN:CG	1:F:252:GLU:HG2	2.23	0.65
1:F:11:VAL:CG2	1:F:78:ALA:HB1	2.27	0.64
1:G:65:SER:H	1:G:68:THR:HB	1.61	0.64
1:B:145:GLY:HA2	1:B:171:LYS:HD2	1.79	0.64
1:D:191:VAL:HG12	1:D:195:VAL:HG22	1.79	0.64
1:A:189:ARG:HG3	1:A:189:ARG:HH11	1.60	0.64
1:H:20:LEU:HD13	1:H:33:GLU:HA	1.78	0.64
1:H:244:THR:OG1	1:H:246:VAL:HG13	1.98	0.63
1:H:11:VAL:CG2	1:H:78:ALA:HB1	2.27	0.63
1:H:25:GLY:HA2	1:H:30:THR:HA	1.79	0.63
1:E:25:GLY:HA3	1:E:146:VAL:HG12	1.81	0.63
1:H:341:ILE:HG13	1:H:362:VAL:HG22	1.80	0.63
1:A:127:ARG:HD2	1:A:133:THR:HG22	1.80	0.63
1:G:19:PRO:HB2	1:G:337:LYS:HE3	1.81	0.63
1:D:240:ILE:HG13	1:D:241:THR:N	2.14	0.63
1:E:8:ILE:HD13	1:E:84:ARG:O	1.99	0.62
1:F:303:THR:HG22	1:F:329:GLU:HG3	1.80	0.62
1:H:339:THR:O	1:H:368:LYS:HD3	2.00	0.62
1:B:136:ASP:C	1:B:354:ILE:HD13	2.25	0.62
1:C:116:ASP:CG	1:C:360:LEU:HD22	2.24	0.62
1:G:43:LEU:HD12	1:G:47:VAL:CG1	2.29	0.62
4:A:412:HOH:O	1:E:207:ARG:HD3	1.98	0.62
1:H:341:ILE:HD11	1:H:362:VAL:HG13	1.81	0.62
1:A:45:ASN:N	1:A:45:ASN:HD22	1.97	0.62
1:B:244:THR:OG1	1:B:246:VAL:HG13	2.00	0.62
1:E:45:ASN:ND2	1:E:47:VAL:H	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LEU:HD13	1:B:279:HIS:CD2	2.34	0.62
1:D:341:ILE:HD12	1:D:364:VAL:HA	1.81	0.62
1:A:92:ILE:HD12	1:A:114:MSE:HE1	1.82	0.61
1:G:92:ILE:HD13	1:G:114:MSE:HE1	1.81	0.61
1:G:187:LEU:O	1:G:187:LEU:HD23	2.00	0.61
1:H:6:LEU:O	1:H:43:LEU:HD22	2.00	0.61
1:B:171:LYS:HE3	4:B:386:HOH:O	2.00	0.61
1:E:141:THR:HG22	1:E:167:SER:OG	2.01	0.61
1:A:145:GLY:HA2	1:A:171:LYS:HD2	1.83	0.61
1:B:25:GLY:HA3	1:B:146:VAL:HG12	1.81	0.61
1:F:26:PHE:CE1	1:F:171:LYS:HE2	2.35	0.61
1:H:23:PRO:HA	1:H:31:SER:O	2.01	0.61
1:H:227:GLN:CG	1:H:252:GLU:HG2	2.22	0.61
1:G:136:ASP:C	1:G:354:ILE:HD13	2.26	0.61
1:G:8:ILE:HD13	1:G:84:ARG:O	2.01	0.61
1:H:236:THR:O	1:H:240:ILE:HG23	2.01	0.61
1:A:339:THR:OG1	1:A:340:TYR:N	2.34	0.60
1:B:149:LEU:O	1:B:153:VAL:HG23	2.01	0.60
1:B:214:LEU:CD1	1:B:240:ILE:HD12	2.30	0.60
1:A:227:GLN:CG	1:A:252:GLU:HG2	2.24	0.60
1:F:15:ILE:HG12	1:F:66:VAL:HG22	1.83	0.60
1:F:149:LEU:O	1:F:153:VAL:HG23	2.00	0.60
1:G:93:MSE:HE2	1:G:93:MSE:HA	1.82	0.60
1:B:207:ARG:HD3	4:F:424:HOH:O	2.01	0.60
1:E:136:ASP:C	1:E:354:ILE:HD13	2.25	0.60
1:G:6:LEU:HG	1:G:86:VAL:HG12	1.83	0.60
1:F:40:SER:HA	1:F:49:GLY:O	2.01	0.60
1:E:237:LEU:O	1:E:240:ILE:HG12	2.02	0.60
1:H:50:TYR:CZ	1:H:364:VAL:HG21	2.37	0.60
1:H:187:LEU:HD23	1:H:187:LEU:O	2.01	0.60
1:H:199:ILE:HD12	1:H:199:ILE:C	2.26	0.60
1:A:99:VAL:HG23	1:A:100:VAL:HG23	1.83	0.59
1:H:191:VAL:O	1:H:193:ASP:N	2.35	0.59
1:A:153:VAL:O	1:A:157:GLU:HG2	2.02	0.59
1:F:21:ILE:HG22	1:F:22:ARG:HG3	1.84	0.59
1:D:45:ASN:ND2	1:D:47:VAL:H	2.00	0.59
1:H:341:ILE:O	1:H:342:VAL:HB	2.03	0.59
1:B:43:LEU:HB2	1:B:45:ASN:ND2	2.16	0.59
1:E:127:ARG:CD	1:E:133:THR:HG22	2.33	0.59
1:F:319:ALA:HB2	1:F:354:ILE:HG12	1.84	0.59
1:G:11:VAL:CG2	1:G:78:ALA:HB1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:VAL:HG12	1:G:195:VAL:HG22	1.84	0.59
1:A:236:THR:O	1:A:240:ILE:HG23	2.02	0.59
1:E:211:LEU:HD23	1:E:240:ILE:HG22	1.85	0.59
1:G:153:VAL:O	1:G:157:GLU:HG2	2.02	0.59
1:A:229:THR:HB	1:A:230:PRO:HD2	1.85	0.59
1:B:127:ARG:CD	1:B:133:THR:HG22	2.33	0.59
1:E:89:LEU:HD12	1:E:283:LEU:HD11	1.85	0.59
1:G:274:LEU:HD13	1:G:279:HIS:CD2	2.38	0.59
1:B:25:GLY:C	1:B:146:VAL:HG12	2.28	0.58
1:B:319:ALA:HB2	1:B:354:ILE:HG12	1.85	0.58
1:B:10:LYS:HE3	1:B:42:HIS:CD2	2.38	0.58
1:C:240:ILE:HG13	1:C:241:THR:N	2.18	0.58
1:F:236:THR:O	1:F:240:ILE:HG23	2.03	0.58
1:A:8:ILE:HD13	1:A:84:ARG:O	2.03	0.58
1:A:261:LEU:HD22	1:A:265:LYS:HE3	1.85	0.58
1:C:43:LEU:HD12	1:C:47:VAL:CG1	2.34	0.58
1:C:176:ASP:OD2	1:C:179:GLU:HG3	2.03	0.58
1:D:43:LEU:HD12	1:D:47:VAL:CG1	2.33	0.58
1:F:25:GLY:C	1:F:146:VAL:HG12	2.29	0.58
1:F:43:LEU:HD12	1:F:47:VAL:CG1	2.33	0.58
1:F:274:LEU:HD13	1:F:279:HIS:CD2	2.39	0.58
1:H:81:LEU:HD23	1:H:114:MSE:HE3	1.84	0.58
1:H:341:ILE:CG1	1:H:362:VAL:HG22	2.33	0.58
1:A:191:VAL:HG12	1:A:195:VAL:HG22	1.86	0.58
1:A:170:LEU:HD11	1:A:187:LEU:HD22	1.86	0.58
1:G:47:VAL:HG11	1:G:121:SER:OG	2.04	0.58
1:G:149:LEU:O	1:G:153:VAL:HG23	2.02	0.58
1:A:187:LEU:C	1:A:187:LEU:HD23	2.29	0.58
1:A:25:GLY:C	1:A:146:VAL:HG12	2.29	0.57
1:E:26:PHE:HE1	1:E:171:LYS:HE2	1.68	0.57
1:D:15:ILE:HG12	1:D:66:VAL:HG22	1.86	0.57
1:E:10:LYS:HE3	1:E:42:HIS:CD2	2.38	0.57
1:F:43:LEU:HB2	1:F:47:VAL:HG12	1.86	0.57
1:F:136:ASP:C	1:F:354:ILE:HD13	2.29	0.57
1:A:6:LEU:HG	1:A:86:VAL:HG12	1.85	0.57
1:B:349:ASP:O	1:B:351:GLN:HG3	2.05	0.57
1:D:171:LYS:HE3	4:D:396:HOH:O	2.04	0.57
1:A:185:ALA:HB1	1:A:189:ARG:HH12	1.69	0.57
1:A:43:LEU:HB2	1:A:45:ASN:HD21	1.70	0.57
1:C:21:ILE:HG12	1:C:337:LYS:HA	1.87	0.57
1:H:341:ILE:HD12	1:H:364:VAL:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:PHE:CE1	1:B:171:LYS:HE2	2.39	0.57
1:B:153:VAL:O	1:B:157:GLU:HG2	2.04	0.57
1:C:229:THR:HB	1:C:230:PRO:HD2	1.87	0.57
1:G:227:GLN:CG	1:G:252:GLU:HG2	2.25	0.57
1:H:45:ASN:ND2	1:H:47:VAL:H	2.03	0.57
1:A:189:ARG:HG3	1:A:189:ARG:NH1	2.19	0.56
1:F:302:ALA:HA	1:F:329:GLU:HG2	1.86	0.56
1:B:68:THR:HG23	1:E:68:THR:OG1	2.05	0.56
1:H:43:LEU:HD12	1:H:47:VAL:CG1	2.35	0.56
1:B:11:VAL:HG21	1:B:78:ALA:CB	2.35	0.56
1:C:26:PHE:CE1	1:C:171:LYS:HE2	2.41	0.56
1:G:144:LEU:HD21	1:G:156:ILE:HG13	1.87	0.56
1:H:274:LEU:HD13	1:H:279:HIS:CD2	2.40	0.56
1:A:43:LEU:HD12	1:A:47:VAL:CG1	2.35	0.56
1:E:227:GLN:CG	1:E:252:GLU:HG2	2.27	0.56
1:D:17:ASP:OD2	1:D:374:ARG:HB2	2.05	0.56
1:D:26:PHE:CE1	1:D:171:LYS:HE2	2.40	0.56
1:D:127:ARG:HE	1:D:133:THR:HG22	1.71	0.56
1:F:341:ILE:HG13	1:F:362:VAL:HG22	1.86	0.56
1:A:78:ALA:N	1:A:79:PRO:HD2	2.20	0.56
1:C:50:TYR:CZ	1:C:364:VAL:HG21	2.41	0.56
1:E:319:ALA:HB2	1:E:354:ILE:HG12	1.87	0.56
1:D:45:ASN:C	1:D:45:ASN:HD22	2.14	0.56
1:H:99:VAL:HG23	1:H:100:VAL:HG23	1.87	0.56
1:A:127:ARG:HE	1:A:133:THR:CG2	2.19	0.55
1:B:62:GLY:O	1:E:102:ARG:HD2	2.06	0.55
1:F:127:ARG:HD2	1:F:133:THR:HG22	1.88	0.55
1:F:169:LYS:HE3	1:F:200:ASP:HB2	1.88	0.55
1:H:104:ARG:O	1:H:280:GLY:HA2	2.06	0.55
1:E:308:PRO:HD2	1:E:340:TYR:CE1	2.42	0.55
1:F:199:ILE:C	1:F:199:ILE:HD12	2.31	0.55
1:D:18:VAL:HG22	1:D:336:LEU:HD22	1.89	0.55
1:A:81:LEU:HD21	1:A:110:VAL:HG13	1.87	0.55
1:F:6:LEU:HB3	1:F:86:VAL:HG12	1.88	0.55
1:B:341:ILE:CG1	1:B:362:VAL:HG22	2.36	0.55
1:G:19:PRO:CB	1:G:337:LYS:HE3	2.36	0.55
1:H:65:SER:O	1:H:69:MSE:HG3	2.07	0.55
1:A:229:THR:HB	1:A:230:PRO:CD	2.37	0.55
1:C:137:LYS:HD2	1:C:351:GLN:NE2	2.22	0.55
1:G:26:PHE:CE1	1:G:171:LYS:HE2	2.41	0.55
1:A:8:ILE:HD11	1:A:86:VAL:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:HD13	1:A:279:HIS:HD2	1.68	0.55
1:B:338:ASP:CG	1:B:339:THR:H	2.15	0.55
1:C:311:THR:OG1	1:C:333:PRO:HD3	2.07	0.54
1:C:20:LEU:HD13	1:C:33:GLU:CA	2.37	0.54
1:C:78:ALA:N	1:C:79:PRO:HD2	2.22	0.54
1:D:8:ILE:HD13	1:D:84:ARG:O	2.08	0.54
1:G:11:VAL:HG21	1:G:78:ALA:HB1	1.90	0.54
1:G:308:PRO:HD2	1:G:340:TYR:CE1	2.42	0.54
1:B:187:LEU:C	1:B:187:LEU:HD23	2.33	0.54
1:E:191:VAL:HG12	1:E:195:VAL:HG22	1.89	0.54
1:G:25:GLY:C	1:G:146:VAL:HG12	2.33	0.54
1:B:40:SER:HA	1:B:49:GLY:O	2.08	0.54
1:B:236:THR:O	1:B:240:ILE:HG23	2.07	0.54
1:D:296:GLY:O	1:H:207:ARG:HB3	2.08	0.54
1:F:176:ASP:OD2	1:F:179:GLU:HG3	2.08	0.54
1:G:236:THR:O	1:G:240:ILE:HG23	2.06	0.54
1:H:126:VAL:HG21	1:H:360:LEU:CD1	2.34	0.54
1:F:13:SER:O	1:F:70:LYS:NZ	2.41	0.54
1:G:127:ARG:HH11	1:G:316:GLN:HE22	1.56	0.54
1:H:92:ILE:HD13	1:H:114:MSE:HE1	1.88	0.54
1:F:187:LEU:C	1:F:187:LEU:HD23	2.33	0.54
1:C:99:VAL:HG23	1:C:100:VAL:HG23	1.88	0.54
1:C:274:LEU:HD13	1:C:279:HIS:CD2	2.42	0.54
1:A:341:ILE:HG13	1:A:362:VAL:CG2	2.38	0.54
1:C:135:ARG:HB3	1:C:135:ARG:NH1	2.21	0.54
1:F:81:LEU:HD23	1:F:114:MSE:HE3	1.90	0.54
1:F:135:ARG:HD2	1:F:138:VAL:HG12	1.89	0.54
1:C:153:VAL:O	1:C:157:GLU:HG2	2.07	0.53
1:C:187:LEU:HD23	1:C:187:LEU:O	2.08	0.53
1:B:135:ARG:HD2	1:B:138:VAL:HG12	1.91	0.53
1:C:5:ASP:O	1:C:44:GLU:HB3	2.09	0.53
1:F:45:ASN:HD21	1:F:47:VAL:CG1	2.11	0.53
1:H:144:LEU:HD12	1:H:144:LEU:N	2.23	0.53
1:A:319:ALA:HB2	1:A:354:ILE:HG12	1.90	0.53
1:F:116:ASP:CG	1:F:360:LEU:HD22	2.33	0.53
1:G:8:ILE:HD11	1:G:86:VAL:HB	1.90	0.53
1:H:214:LEU:HD13	1:H:240:ILE:HD12	1.89	0.53
1:H:339:THR:OG1	1:H:340:TYR:N	2.41	0.53
1:B:187:LEU:HD23	1:B:187:LEU:O	2.08	0.53
1:B:274:LEU:C	1:B:274:LEU:HD12	2.33	0.53
1:F:156:ILE:HG21	1:F:191:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASN:HD21	1:A:47:VAL:CG1	2.15	0.53
1:B:68:THR:HG23	1:E:68:THR:HG23	1.89	0.53
1:C:89:LEU:HD21	1:C:115:HIS:CD2	2.44	0.53
1:D:127:ARG:HE	1:D:133:THR:CG2	2.21	0.53
1:F:45:ASN:ND2	1:F:47:VAL:H	2.06	0.53
1:G:13:SER:HB2	1:G:37:LEU:HD11	1.89	0.53
1:A:127:ARG:CD	1:A:133:THR:HG22	2.39	0.53
1:D:20:LEU:HD13	1:D:33:GLU:CA	2.37	0.53
1:D:156:ILE:HG21	1:D:191:VAL:HG11	1.91	0.53
1:G:341:ILE:HD11	1:G:362:VAL:HG13	1.90	0.53
1:C:199:ILE:HD12	1:C:199:ILE:C	2.34	0.53
1:H:274:LEU:HD13	1:H:279:HIS:HD2	1.73	0.53
1:C:137:LYS:CE	1:C:351:GLN:HE22	2.22	0.53
1:G:92:ILE:HG22	1:G:93:MSE:CE	2.39	0.53
1:B:120:ARG:HG2	1:B:120:ARG:HH11	1.72	0.52
1:F:45:ASN:C	1:F:45:ASN:HD22	2.16	0.52
1:A:156:ILE:HG21	1:A:191:VAL:HG11	1.91	0.52
1:F:15:ILE:HG12	1:F:66:VAL:CG2	2.39	0.52
1:G:354:ILE:HD12	1:G:354:ILE:N	2.24	0.52
1:E:187:LEU:HD23	1:E:187:LEU:C	2.34	0.52
1:C:341:ILE:HG13	1:C:362:VAL:HG22	1.90	0.52
1:E:43:LEU:HD12	1:E:47:VAL:HG11	1.89	0.52
1:F:41:VAL:HG23	1:F:113:ALA:HB1	1.91	0.52
1:B:227:GLN:CG	1:B:252:GLU:HG2	2.29	0.52
1:C:187:LEU:HD23	1:C:187:LEU:C	2.35	0.52
1:D:137:LYS:N	1:D:354:ILE:HD13	2.25	0.52
1:F:207:ARG:HD3	4:H:476:HOH:O	2.09	0.52
1:G:187:LEU:HD23	1:G:187:LEU:C	2.35	0.52
1:H:10:LYS:HE3	1:H:42:HIS:CD2	2.45	0.52
1:C:137:LYS:N	1:C:354:ILE:HD13	2.25	0.52
1:C:227:GLN:CG	1:C:252:GLU:HG2	2.29	0.52
1:D:40:SER:HB3	1:D:50:TYR:CE1	2.44	0.52
1:H:147:LEU:H	1:H:183:ARG:NH1	2.08	0.52
1:A:5:ASP:O	1:A:44:GLU:HB3	2.10	0.52
1:A:47:VAL:HG11	1:A:121:SER:OG	2.09	0.52
1:B:189:ARG:HG3	1:B:189:ARG:HH11	1.73	0.52
1:B:238:ARG:HD3	1:B:267:GLN:O	2.10	0.52
1:F:127:ARG:HE	1:F:133:THR:CG2	2.23	0.52
1:H:81:LEU:HD21	1:H:110:VAL:HG13	1.91	0.52
1:A:251:ASP:HB3	1:A:252:GLU:OE2	2.10	0.52
1:F:20:LEU:HD13	1:F:33:GLU:CA	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:GLU:OE1	1:G:105:TYR:HB2	2.10	0.52
1:H:341:ILE:O	1:H:363:ASP:O	2.28	0.52
1:A:45:ASN:ND2	1:A:45:ASN:N	2.58	0.51
1:E:11:VAL:HG21	1:E:78:ALA:CB	2.38	0.51
1:H:185:ALA:O	1:H:188:ALA:HB3	2.09	0.51
1:B:104:ARG:O	1:B:280:GLY:HA2	2.10	0.51
1:B:169:LYS:HE3	1:B:200:ASP:HB2	1.93	0.51
1:D:201:ILE:HB	1:D:228:PRO:HA	1.92	0.51
1:A:45:ASN:ND2	1:A:45:ASN:H	2.08	0.51
1:B:20:LEU:HD13	1:B:33:GLU:CA	2.39	0.51
1:B:47:VAL:HG11	1:B:121:SER:OG	2.10	0.51
1:D:187:LEU:C	1:D:187:LEU:HD23	2.34	0.51
1:H:9:GLN:HE21	1:H:44:GLU:HB2	1.76	0.51
1:D:187:LEU:HD23	1:D:187:LEU:O	2.11	0.51
1:G:126:VAL:HG21	1:G:360:LEU:HD13	1.92	0.51
1:H:217:LEU:HB3	1:H:222:VAL:HG21	1.92	0.51
1:D:65:SER:H	1:D:68:THR:HB	1.76	0.51
1:D:244:THR:OG1	1:D:246:VAL:HG13	2.10	0.51
1:G:91:GLY:HA2	1:H:134:VAL:HG22	1.92	0.51
1:G:333:PRO:HG2	1:G:345:PHE:CE2	2.45	0.51
1:A:65:SER:H	1:A:68:THR:HB	1.76	0.51
1:D:240:ILE:HD11	1:D:248:VAL:CG2	2.38	0.51
1:D:274:LEU:HD13	1:D:279:HIS:CD2	2.46	0.51
1:H:8:ILE:HD11	1:H:86:VAL:CB	2.41	0.51
1:F:11:VAL:HG23	1:F:78:ALA:HB1	1.91	0.51
1:H:302:ALA:HA	1:H:329:GLU:HG2	1.91	0.51
1:A:125:PRO:HD2	1:A:128:ASP:OD2	2.11	0.51
1:C:50:TYR:CE2	1:C:364:VAL:HG21	2.46	0.51
1:C:65:SER:H	1:C:68:THR:HB	1.76	0.51
1:E:126:VAL:HG21	1:E:360:LEU:CD1	2.40	0.51
1:E:43:LEU:HD12	1:E:47:VAL:HG13	1.92	0.50
1:F:40:SER:HB3	1:F:50:TYR:CE1	2.46	0.50
1:D:6:LEU:HG	1:D:86:VAL:HG12	1.91	0.50
1:B:111:ASP:O	1:B:115:HIS:HD2	1.95	0.50
1:B:127:ARG:HE	1:B:133:THR:CG2	2.24	0.50
1:B:25:GLY:CA	1:B:146:VAL:HG12	2.41	0.50
1:C:6:LEU:HG	1:C:86:VAL:HG12	1.92	0.50
1:E:341:ILE:HG13	1:E:362:VAL:HG22	1.94	0.50
1:F:229:THR:HB	1:F:230:PRO:CD	2.42	0.50
1:F:244:THR:OG1	1:F:246:VAL:HG13	2.11	0.50
1:H:229:THR:HB	1:H:230:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ALA:O	1:B:182:ARG:HD3	2.11	0.50
1:G:115:HIS:CD2	1:G:282:LEU:HD12	2.46	0.50
1:G:229:THR:HB	1:G:230:PRO:HD2	1.92	0.50
1:C:27:ALA:CB	1:C:204:ARG:HG3	2.41	0.50
1:D:185:ALA:O	1:D:189:ARG:HG3	2.11	0.50
1:E:242:ARG:NH2	4:E:715:HOH:O	2.45	0.50
1:H:45:ASN:ND2	1:H:45:ASN:C	2.67	0.50
1:C:238:ARG:HD3	1:C:267:GLN:O	2.12	0.50
1:D:309:ILE:HD11	1:D:364:VAL:HG12	1.93	0.50
1:F:135:ARG:HH11	1:F:135:ARG:HB3	1.76	0.50
1:F:339:THR:OG1	1:F:340:TYR:N	2.44	0.50
1:G:170:LEU:HD11	1:G:187:LEU:HD22	1.94	0.50
1:H:8:ILE:HD12	1:H:8:ILE:N	2.27	0.50
1:D:251:ASP:HB3	1:D:252:GLU:OE2	2.12	0.49
1:H:276:THR:HA	1:H:285:SER:OG	2.12	0.49
1:D:229:THR:HB	1:D:230:PRO:HD2	1.94	0.49
1:E:45:ASN:HD22	1:E:47:VAL:H	1.59	0.49
1:E:127:ARG:HE	1:E:133:THR:CG2	2.25	0.49
1:D:169:LYS:HE3	1:D:200:ASP:HB2	1.93	0.49
1:E:226:GLU:O	1:E:227:GLN:C	2.56	0.49
1:F:8:ILE:HD11	1:F:86:VAL:HB	1.92	0.49
1:F:43:LEU:HD12	1:F:47:VAL:HG11	1.95	0.49
1:G:229:THR:HB	1:G:230:PRO:CD	2.42	0.49
1:C:139:ASP:HA	1:C:351:GLN:HG2	1.93	0.49
1:H:145:GLY:HA2	1:H:171:LYS:HD2	1.93	0.49
1:B:274:LEU:HD13	1:B:279:HIS:HD2	1.76	0.49
1:C:303:THR:HG22	1:C:329:GLU:HG3	1.93	0.49
1:C:92:ILE:HD12	1:C:114:MSE:CE	2.33	0.49
1:E:8:ILE:HD11	1:E:86:VAL:CA	2.42	0.49
1:H:54:VAL:HG11	1:H:306:GLU:HA	1.94	0.49
1:H:147:LEU:H	1:H:183:ARG:HH12	1.61	0.49
1:C:274:LEU:HD12	1:C:274:LEU:C	2.37	0.49
1:F:11:VAL:HG21	1:F:78:ALA:HB1	1.93	0.49
1:A:21:ILE:HG12	1:A:337:LYS:HA	1.95	0.49
1:B:191:VAL:HG12	1:B:195:VAL:HG22	1.93	0.49
1:F:229:THR:HB	1:F:230:PRO:HD2	1.93	0.49
1:B:88:GLU:O	1:B:92:ILE:HG13	2.13	0.49
1:C:59:PRO:HD3	1:C:65:SER:HB3	1.95	0.49
1:F:25:GLY:HA3	1:F:146:VAL:HG12	1.94	0.49
1:F:341:ILE:CG1	1:F:362:VAL:HG22	2.42	0.49
1:G:26:PHE:HE1	1:G:171:LYS:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:238:ARG:HD3	1:G:267:GLN:O	2.13	0.49
1:H:331:PHE:CD1	1:H:331:PHE:C	2.90	0.49
1:A:116:ASP:CG	1:A:360:LEU:HD22	2.37	0.49
1:D:127:ARG:HH11	1:D:316:GLN:HE22	1.61	0.49
1:G:313:ALA:HA	1:G:360:LEU:HD12	1.94	0.49
1:A:25:GLY:O	1:A:146:VAL:HG12	2.12	0.48
1:F:45:ASN:ND2	1:F:47:VAL:HG12	2.11	0.48
1:A:116:ASP:OD1	1:A:360:LEU:HD22	2.14	0.48
1:A:308:PRO:HD2	1:A:340:TYR:CE1	2.48	0.48
1:B:311:THR:O	1:B:315:LEU:HG	2.14	0.48
1:C:11:VAL:CG2	1:C:78:ALA:HB1	2.43	0.48
1:D:47:VAL:HG11	1:D:121:SER:OG	2.13	0.48
1:D:227:GLN:CG	1:D:252:GLU:HG2	2.34	0.48
1:E:143:ALA:HB3	1:E:331:PHE:CZ	2.48	0.48
1:A:240:ILE:HG13	1:A:241:THR:N	2.27	0.48
1:E:225:PHE:CE2	1:E:246:VAL:HG11	2.49	0.48
1:F:37:LEU:HB2	1:F:66:VAL:HG23	1.95	0.48
1:H:127:ARG:HB3	1:H:316:GLN:NE2	2.28	0.48
1:B:93:MSE:HE1	1:B:96:LEU:HD11	1.96	0.48
1:B:116:ASP:OD1	1:B:360:LEU:HD22	2.13	0.48
1:C:201:ILE:HD13	1:C:205:TRP:CD2	2.49	0.48
1:E:78:ALA:N	1:E:79:PRO:HD2	2.29	0.48
1:E:229:THR:HB	1:E:230:PRO:HD2	1.95	0.48
1:F:135:ARG:HB3	1:F:135:ARG:NH1	2.29	0.48
1:G:176:ASP:OD2	1:G:178:ALA:HB3	2.14	0.48
1:B:251:ASP:HB3	1:B:252:GLU:OE2	2.13	0.48
1:F:78:ALA:N	1:F:79:PRO:HD2	2.29	0.48
1:G:198:ARG:HG3	1:G:224:LEU:HB3	1.94	0.48
1:F:93:MSE:HE1	1:F:96:LEU:HD11	1.96	0.48
1:F:127:ARG:CD	1:F:133:THR:HG22	2.44	0.48
1:B:331:PHE:CD1	1:B:331:PHE:C	2.92	0.48
1:E:8:ILE:HD12	1:E:8:ILE:N	2.29	0.48
1:G:92:ILE:CD1	1:G:114:MSE:HE1	2.43	0.48
1:H:40:SER:HA	1:H:49:GLY:O	2.13	0.48
1:A:137:LYS:N	1:A:354:ILE:HD13	2.29	0.47
1:D:304:SER:O	1:D:305:LEU:HB2	2.13	0.47
1:A:125:PRO:HB3	1:A:127:ARG:NH1	2.29	0.47
1:F:18:VAL:O	1:F:33:GLU:HB2	2.15	0.47
1:A:11:VAL:HG21	1:A:78:ALA:CB	2.35	0.47
1:B:157:GLU:OE1	1:B:194:ARG:NH2	2.45	0.47
1:C:104:ARG:O	1:C:280:GLY:HA2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:THR:O	1:D:368:LYS:HD3	2.13	0.47
1:A:276:THR:HA	1:A:285:SER:OG	2.15	0.47
1:C:136:ASP:C	1:C:354:ILE:HD13	2.39	0.47
1:E:84:ARG:HD2	4:E:443:HOH:O	2.14	0.47
1:G:240:ILE:HD11	1:G:248:VAL:CG2	2.43	0.47
1:H:110:VAL:O	1:H:114:MSE:HG3	2.14	0.47
1:A:127:ARG:HE	1:A:133:THR:HG22	1.80	0.47
1:F:341:ILE:O	1:F:342:VAL:HB	2.14	0.47
1:A:11:VAL:HG12	1:A:41:VAL:HG22	1.96	0.47
1:B:43:LEU:HD12	1:B:47:VAL:CG1	2.44	0.47
1:B:93:MSE:HE2	1:B:93:MSE:CA	2.42	0.47
1:C:229:THR:HB	1:C:230:PRO:CD	2.45	0.47
1:F:239:GLU:HA	1:F:242:ARG:HE	1.80	0.47
1:G:125:PRO:HD2	1:G:128:ASP:OD2	2.15	0.47
1:G:144:LEU:N	1:G:144:LEU:HD12	2.29	0.47
1:G:341:ILE:O	1:G:363:ASP:O	2.33	0.47
1:B:120:ARG:HG2	1:B:120:ARG:NH1	2.30	0.47
1:E:8:ILE:HD11	1:E:86:VAL:CB	2.45	0.47
1:F:156:ILE:O	1:F:160:ILE:HG13	2.14	0.47
1:B:127:ARG:HE	1:B:133:THR:HG21	1.79	0.47
1:B:229:THR:HB	1:B:230:PRO:HD2	1.97	0.47
1:C:141:THR:HG23	1:C:328:THR:O	2.14	0.47
1:D:299:CYS:HB2	1:D:323:ALA:O	2.14	0.47
1:F:299:CYS:HB2	1:F:323:ALA:O	2.14	0.47
1:H:238:ARG:HE	1:H:242:ARG:HH11	1.61	0.47
1:H:369:VAL:O	1:H:373:THR:OG1	2.29	0.47
1:C:137:LYS:HD2	1:C:351:GLN:HE22	1.80	0.47
1:C:149:LEU:O	1:C:153:VAL:HG23	2.15	0.47
1:C:256:THR:OG1	1:C:259:GLU:HG3	2.15	0.47
1:G:137:LYS:N	1:G:354:ILE:HD13	2.30	0.47
1:G:341:ILE:HD12	1:G:364:VAL:HA	1.97	0.47
1:C:69:MSE:O	1:C:73:VAL:HG23	2.15	0.46
1:C:144:LEU:HD12	1:C:144:LEU:N	2.30	0.46
1:D:156:ILE:O	1:D:160:ILE:HG13	2.16	0.46
1:D:201:ILE:HD12	1:D:228:PRO:CB	2.45	0.46
1:E:238:ARG:HD3	1:E:267:GLN:O	2.15	0.46
1:G:104:ARG:O	1:G:280:GLY:HA2	2.15	0.46
1:G:289:ALA:HB1	1:G:323:ALA:HB3	1.96	0.46
1:H:136:ASP:C	1:H:354:ILE:HD13	2.40	0.46
1:B:36:ILE:CG2	1:B:52:GLU:HG2	2.46	0.46
1:C:68:THR:OG1	1:H:68:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:VAL:CG2	1:D:336:LEU:HD22	2.46	0.46
1:D:45:ASN:ND2	1:D:45:ASN:C	2.73	0.46
1:D:229:THR:HB	1:D:230:PRO:CD	2.44	0.46
1:B:189:ARG:HG3	1:B:189:ARG:NH1	2.30	0.46
1:C:319:ALA:HB2	1:C:354:ILE:HG12	1.97	0.46
1:G:331:PHE:O	1:G:332:GLY:C	2.59	0.46
1:D:8:ILE:HD11	1:D:86:VAL:CA	2.45	0.46
1:F:92:ILE:CD1	1:F:114:MSE:HE1	2.41	0.46
1:B:45:ASN:N	1:B:45:ASN:HD22	2.12	0.46
1:E:126:VAL:HG21	1:E:360:LEU:HD12	1.97	0.46
1:E:308:PRO:HD2	1:E:340:TYR:CZ	2.51	0.46
1:F:45:ASN:ND2	1:F:45:ASN:C	2.73	0.46
1:G:49:GLY:HA2	1:G:116:ASP:OD2	2.16	0.46
1:G:339:THR:OG1	1:G:340:TYR:N	2.49	0.46
1:B:11:VAL:HG23	1:B:78:ALA:HB1	1.95	0.46
1:B:179:GLU:HG2	1:B:182:ARG:NH2	2.30	0.46
1:B:226:GLU:O	1:B:227:GLN:C	2.58	0.46
1:C:302:ALA:HA	1:C:329:GLU:HG2	1.98	0.46
1:D:214:LEU:N	1:D:215:PRO:CD	2.78	0.46
1:G:225:PHE:CE2	1:G:246:VAL:CG1	2.99	0.46
1:H:319:ALA:HB2	1:H:354:ILE:HG12	1.97	0.46
1:A:322:LYS:O	1:A:322:LYS:HD3	2.16	0.46
1:B:160:ILE:O	1:B:164:GLY:HA2	2.16	0.46
1:D:54:VAL:HG11	1:D:306:GLU:HA	1.98	0.46
1:E:81:LEU:HG	1:E:92:ILE:HG21	1.98	0.46
1:E:229:THR:HB	1:E:230:PRO:CD	2.44	0.46
1:H:191:VAL:HG12	1:H:195:VAL:HG22	1.97	0.46
1:E:339:THR:OG1	1:E:340:TYR:N	2.49	0.46
1:G:37:LEU:HB2	1:G:66:VAL:HG23	1.97	0.46
1:G:214:LEU:N	1:G:215:PRO:CD	2.79	0.46
1:E:274:LEU:HD13	1:E:279:HIS:CD2	2.51	0.46
1:F:127:ARG:HE	1:F:133:THR:HG22	1.79	0.46
1:G:92:ILE:HG22	1:G:93:MSE:HE2	1.97	0.46
1:C:135:ARG:HH11	1:C:135:ARG:CB	2.23	0.46
1:G:16:LEU:HD23	1:G:373:THR:HA	1.97	0.46
1:G:41:VAL:HG23	1:G:113:ALA:CB	2.46	0.46
1:G:240:ILE:HG13	1:G:241:THR:N	2.31	0.46
1:C:207:ARG:HB3	1:G:296:GLY:O	2.16	0.45
1:G:20:LEU:HD13	1:G:33:GLU:HA	1.97	0.45
1:G:126:VAL:HB	1:G:316:GLN:HG3	1.98	0.45
1:A:199:ILE:C	1:A:199:ILE:HD12	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LYS:HE3	1:C:200:ASP:HB2	1.97	0.45
1:D:43:LEU:HB2	1:D:47:VAL:HG12	1.98	0.45
1:E:201:ILE:HB	1:E:228:PRO:HA	1.98	0.45
1:F:93:MSE:HA	1:F:93:MSE:CE	2.42	0.45
1:H:289:ALA:HB1	1:H:323:ALA:HB3	1.98	0.45
1:A:155:GLU:O	1:A:159:ARG:HG2	2.16	0.45
1:B:8:ILE:HD13	1:B:84:ARG:O	2.16	0.45
1:C:11:VAL:HG12	1:C:41:VAL:HG22	1.97	0.45
1:D:26:PHE:HE1	1:D:171:LYS:HE2	1.81	0.45
1:D:226:GLU:CD	1:D:249:MSE:HE3	2.41	0.45
1:E:8:ILE:HD11	1:E:86:VAL:HB	1.98	0.45
1:F:309:ILE:HD11	1:F:341:ILE:HD11	1.98	0.45
1:G:370:ASN:N	1:G:370:ASN:HD22	2.13	0.45
1:A:240:ILE:HD11	1:A:248:VAL:HG22	1.99	0.45
1:H:8:ILE:HD13	1:H:84:ARG:O	2.16	0.45
1:A:214:LEU:N	1:A:215:PRO:CD	2.80	0.45
1:B:68:THR:HG23	1:E:68:THR:CG2	2.46	0.45
1:C:40:SER:HA	1:C:49:GLY:O	2.17	0.45
1:C:127:ARG:HH11	1:C:316:GLN:HE22	1.65	0.45
1:H:47:VAL:HG22	1:H:48:ILE:N	2.32	0.45
1:B:274:LEU:C	1:B:274:LEU:CD1	2.89	0.45
1:C:27:ALA:HB3	1:C:204:ARG:HG3	1.98	0.45
1:D:21:ILE:HG22	1:D:22:ARG:HG3	1.98	0.45
1:E:146:VAL:O	1:E:146:VAL:HG13	2.15	0.45
1:G:45:ASN:C	1:G:45:ASN:HD22	2.24	0.45
1:G:126:VAL:HG23	1:G:359:GLY:C	2.42	0.45
1:G:194:ARG:HG3	1:G:194:ARG:HH11	1.81	0.45
1:B:116:ASP:CG	1:B:360:LEU:HD22	2.42	0.45
1:D:130:LEU:HD11	1:D:282:LEU:HD13	1.98	0.45
1:G:274:LEU:C	1:G:274:LEU:HD12	2.41	0.45
1:H:78:ALA:N	1:H:79:PRO:HD2	2.32	0.45
1:D:44:GLU:C	1:D:46:GLY:H	2.25	0.45
1:E:251:ASP:HB3	1:E:252:GLU:OE2	2.17	0.45
1:F:214:LEU:N	1:F:215:PRO:CD	2.80	0.45
1:G:91:GLY:CA	1:H:134:VAL:HG22	2.47	0.45
1:C:93:MSE:HA	1:C:93:MSE:HE2	1.97	0.45
1:F:251:ASP:HB3	1:F:252:GLU:OE2	2.17	0.45
1:G:309:ILE:HG12	1:G:341:ILE:HD13	1.99	0.45
1:A:43:LEU:HD12	1:A:47:VAL:HG11	1.99	0.44
1:A:274:LEU:HD12	1:A:274:LEU:C	2.42	0.44
1:C:341:ILE:CG1	1:C:362:VAL:HG22	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLU:O	1:D:159:ARG:HG2	2.16	0.44
1:E:306:GLU:HB3	1:E:310:GLY:HA3	1.99	0.44
1:H:256:THR:OG1	1:H:259:GLU:HG3	2.17	0.44
1:H:303:THR:HG22	1:H:329:GLU:CD	2.42	0.44
1:A:43:LEU:HB2	1:A:47:VAL:CG1	2.48	0.44
1:H:120:ARG:HH11	1:H:120:ARG:HG2	1.82	0.44
1:C:304:SER:O	1:C:305:LEU:HB2	2.17	0.44
1:G:303:THR:HG22	1:G:329:GLU:HG3	2.00	0.44
1:A:143:ALA:HB3	1:A:331:PHE:CZ	2.53	0.44
1:A:240:ILE:HD11	1:A:248:VAL:CG2	2.48	0.44
1:B:194:ARG:HG3	1:B:194:ARG:HH11	1.81	0.44
1:B:309:ILE:HD11	1:B:341:ILE:HD11	1.99	0.44
1:C:126:VAL:HG21	1:C:360:LEU:HD13	1.99	0.44
1:C:170:LEU:HD11	1:C:187:LEU:HD22	1.98	0.44
1:D:132:GLY:O	1:D:320:SER:HB3	2.18	0.44
1:D:302:ALA:HA	1:D:329:GLU:HG2	2.00	0.44
1:E:127:ARG:NE	1:E:133:THR:HG22	2.32	0.44
1:E:338:ASP:CG	1:E:339:THR:H	2.25	0.44
1:H:45:ASN:HD22	1:H:46:GLY:N	2.14	0.44
1:H:146:VAL:HG13	1:H:146:VAL:O	2.16	0.44
1:B:169:LYS:HE3	1:B:200:ASP:CB	2.48	0.44
1:B:304:SER:HB2	1:B:306:GLU:OE2	2.16	0.44
1:C:45:ASN:HD21	1:C:47:VAL:CG1	2.01	0.44
1:D:146:VAL:O	1:D:146:VAL:HG13	2.17	0.44
1:F:187:LEU:HD23	1:F:187:LEU:O	2.17	0.44
1:G:198:ARG:HD2	1:G:198:ARG:N	2.33	0.44
1:H:47:VAL:HG11	1:H:121:SER:OG	2.17	0.44
1:A:69:MSE:O	1:A:73:VAL:HG23	2.18	0.44
1:B:176:ASP:OD2	1:B:179:GLU:HG3	2.17	0.44
1:C:138:VAL:HG13	1:C:354:ILE:HD11	2.00	0.44
1:C:251:ASP:HB3	1:C:252:GLU:OE2	2.17	0.44
1:D:135:ARG:HD2	1:D:138:VAL:HG12	1.98	0.44
1:G:199:ILE:C	1:G:199:ILE:HD12	2.42	0.44
1:A:127:ARG:NE	1:A:133:THR:HG22	2.32	0.44
1:B:25:GLY:HA3	1:B:146:VAL:CG1	2.47	0.44
1:D:11:VAL:HG21	1:D:78:ALA:CB	2.45	0.44
1:F:143:ALA:HA	1:F:169:LYS:O	2.18	0.44
1:C:146:VAL:HG13	1:C:146:VAL:O	2.17	0.44
1:D:242:ARG:NH2	4:D:772:HOH:O	2.51	0.44
1:G:86:VAL:HG23	1:G:114:MSE:HE2	2.00	0.44
1:A:41:VAL:HG23	1:A:113:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:THR:OG1	1:A:246:VAL:HG13	2.18	0.44
1:B:311:THR:OG1	1:B:333:PRO:HD3	2.18	0.44
1:H:226:GLU:O	1:H:227:GLN:C	2.61	0.44
1:H:251:ASP:HB3	1:H:252:GLU:OE2	2.18	0.44
1:A:309:ILE:CD1	1:A:341:ILE:HD11	2.48	0.43
1:D:78:ALA:N	1:D:79:PRO:HD2	2.32	0.43
1:H:169:LYS:HE3	1:H:200:ASP:HB2	1.99	0.43
1:A:15:ILE:HG12	1:A:66:VAL:CG2	2.48	0.43
1:B:22:ARG:HG2	1:B:22:ARG:HH11	1.83	0.43
1:B:26:PHE:HE1	1:B:171:LYS:HE2	1.83	0.43
1:B:341:ILE:O	1:B:341:ILE:HG23	2.18	0.43
1:B:341:ILE:O	1:B:342:VAL:HB	2.18	0.43
1:C:11:VAL:HG21	1:C:78:ALA:HB1	2.01	0.43
1:C:225:PHE:CE2	1:C:246:VAL:HG11	2.54	0.43
1:C:249:MSE:HA	1:C:271:VAL:O	2.19	0.43
1:G:309:ILE:HD11	1:G:341:ILE:HD11	2.00	0.43
1:H:42:HIS:CE1	1:H:48:ILE:HD13	2.53	0.43
1:A:81:LEU:HD21	1:A:110:VAL:CG1	2.48	0.43
1:C:341:ILE:O	1:C:341:ILE:HG23	2.18	0.43
1:D:89:LEU:HD22	1:D:114:MSE:HB3	2.00	0.43
1:E:156:ILE:HG21	1:E:191:VAL:HG11	2.00	0.43
1:F:341:ILE:O	1:F:341:ILE:HG23	2.18	0.43
1:G:269:ALA:O	1:G:297:LEU:HD22	2.18	0.43
1:H:303:THR:HG22	1:H:329:GLU:OE2	2.18	0.43
1:C:8:ILE:HD12	1:C:84:ARG:O	2.19	0.43
1:C:226:GLU:O	1:C:227:GLN:C	2.62	0.43
1:E:104:ARG:O	1:E:280:GLY:HA2	2.18	0.43
1:E:127:ARG:HE	1:E:133:THR:HG22	1.83	0.43
1:F:127:ARG:NE	1:F:133:THR:HG22	2.34	0.43
1:F:331:PHE:CD1	1:F:331:PHE:C	2.96	0.43
1:G:365:ASP:OD1	1:G:367:ASP:HB2	2.17	0.43
1:H:229:THR:HB	1:H:230:PRO:CD	2.48	0.43
1:A:86:VAL:HA	1:A:114:MSE:HE3	2.00	0.43
1:C:18:VAL:HG13	1:C:336:LEU:HD22	2.00	0.43
1:E:156:ILE:O	1:E:160:ILE:HG13	2.18	0.43
1:H:11:VAL:HG23	1:H:78:ALA:HB1	2.01	0.43
1:H:217:LEU:HB3	1:H:222:VAL:CG2	2.48	0.43
1:A:8:ILE:HD11	1:A:86:VAL:CB	2.48	0.43
1:B:89:LEU:HD12	1:B:89:LEU:C	2.43	0.43
1:C:77:LEU:HD22	1:C:96:LEU:HD13	2.01	0.43
1:D:8:ILE:N	1:D:8:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:THR:OG1	1:E:246:VAL:HG13	2.18	0.43
1:F:8:ILE:HD11	1:F:86:VAL:CB	2.49	0.43
1:F:274:LEU:HD13	1:F:279:HIS:HD2	1.80	0.43
1:G:278:LYS:HE3	1:G:279:HIS:CE1	2.54	0.43
1:G:339:THR:O	1:G:368:LYS:HD3	2.19	0.43
1:H:135:ARG:HD2	1:H:138:VAL:HG12	2.01	0.43
1:A:20:LEU:HD13	1:A:33:GLU:CA	2.45	0.43
1:A:135:ARG:HD2	1:A:138:VAL:HG12	2.01	0.43
1:B:207:ARG:HB3	1:F:296:GLY:O	2.18	0.43
1:E:240:ILE:HD11	1:E:248:VAL:HG21	2.00	0.43
1:E:304:SER:O	1:E:305:LEU:HB2	2.17	0.43
1:G:156:ILE:HG23	1:G:168:PHE:CE2	2.53	0.43
1:A:8:ILE:N	1:A:8:ILE:HD12	2.34	0.43
1:D:43:LEU:HD12	1:D:47:VAL:HG11	1.99	0.43
1:F:127:ARG:H	1:F:316:GLN:HE21	1.66	0.43
1:F:179:GLU:HG2	1:F:182:ARG:NH2	2.34	0.43
1:F:180:ASP:OD1	1:F:183:ARG:NH2	2.45	0.43
1:G:40:SER:HA	1:G:49:GLY:O	2.19	0.43
1:G:119:ALA:HB3	1:G:359:GLY:HA2	2.01	0.43
1:G:120:ARG:HG3	1:G:359:GLY:HA3	1.99	0.43
1:C:8:ILE:CD1	1:C:84:ARG:O	2.67	0.43
1:C:45:ASN:C	1:C:45:ASN:HD22	2.26	0.43
1:C:86:VAL:HA	1:C:114:MSE:HE3	2.01	0.43
1:C:137:LYS:CD	1:C:351:GLN:HE22	2.32	0.43
1:D:126:VAL:HG23	1:D:359:GLY:C	2.44	0.43
1:F:201:ILE:HB	1:F:228:PRO:HA	2.01	0.43
1:G:249:MSE:HA	1:G:271:VAL:O	2.19	0.43
1:H:26:PHE:CE1	1:H:171:LYS:HE2	2.54	0.43
1:H:341:ILE:CD1	1:H:362:VAL:HG13	2.47	0.43
1:A:43:LEU:HB2	1:A:47:VAL:HG13	2.00	0.42
1:A:127:ARG:H	1:A:316:GLN:NE2	2.17	0.42
1:A:169:LYS:HE3	1:A:200:ASP:HB2	2.01	0.42
1:A:238:ARG:HD3	1:A:267:GLN:O	2.19	0.42
1:A:331:PHE:O	1:A:332:GLY:C	2.61	0.42
1:C:289:ALA:HB1	1:C:323:ALA:HB3	2.01	0.42
1:E:144:LEU:N	1:E:144:LEU:HD12	2.33	0.42
1:F:303:THR:HG22	1:F:329:GLU:CG	2.48	0.42
1:G:11:VAL:HG23	1:G:78:ALA:HB1	1.99	0.42
1:H:8:ILE:HD11	1:H:86:VAL:CA	2.49	0.42
1:H:127:ARG:HD2	1:H:133:THR:HG22	2.00	0.42
1:H:308:PRO:HD2	1:H:340:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HD21	1:A:115:HIS:CD2	2.54	0.42
1:B:296:GLY:O	1:D:207:ARG:HB3	2.18	0.42
1:E:341:ILE:HG23	1:E:341:ILE:O	2.18	0.42
1:F:104:ARG:HE	1:F:256:THR:HG22	1.84	0.42
1:G:6:LEU:HD11	1:G:121:SER:CB	2.50	0.42
1:A:313:ALA:HA	1:A:360:LEU:HD12	2.01	0.42
1:B:45:ASN:ND2	1:B:45:ASN:N	2.66	0.42
1:B:199:ILE:C	1:B:199:ILE:HD12	2.44	0.42
1:C:8:ILE:HD11	1:C:86:VAL:CA	2.49	0.42
1:C:214:LEU:N	1:C:215:PRO:CD	2.82	0.42
1:H:73:VAL:HA	1:H:77:LEU:HB2	2.00	0.42
1:H:160:ILE:O	1:H:164:GLY:HA2	2.18	0.42
1:F:86:VAL:C	1:F:88:GLU:H	2.27	0.42
1:F:168:PHE:HE2	1:F:195:VAL:HG11	1.85	0.42
1:G:225:PHE:CE2	1:G:246:VAL:HG13	2.54	0.42
1:G:359:GLY:C	1:G:361:GLY:N	2.76	0.42
1:A:8:ILE:HD11	1:A:86:VAL:CA	2.49	0.42
1:D:37:LEU:HB2	1:D:66:VAL:HG23	2.01	0.42
1:D:274:LEU:HD13	1:D:279:HIS:HD2	1.85	0.42
1:E:341:ILE:HD11	1:E:362:VAL:HG13	2.02	0.42
1:G:78:ALA:N	1:G:79:PRO:HD2	2.34	0.42
1:G:89:LEU:HD13	1:G:114:MSE:CB	2.49	0.42
1:H:354:ILE:N	1:H:354:ILE:HD12	2.34	0.42
1:A:104:ARG:CZ	4:A:391:HOH:O	2.68	0.42
1:B:93:MSE:HA	1:B:93:MSE:CE	2.47	0.42
1:C:25:GLY:HA2	1:C:30:THR:HA	2.00	0.42
1:C:49:GLY:HA3	1:C:117:ALA:HB2	2.00	0.42
1:C:299:CYS:HB2	1:C:323:ALA:O	2.18	0.42
1:E:225:PHE:CE2	1:E:246:VAL:CG1	3.02	0.42
1:E:261:LEU:HD13	1:E:265:LYS:HE3	2.02	0.42
1:G:226:GLU:O	1:G:227:GLN:C	2.62	0.42
1:H:201:ILE:HB	1:H:228:PRO:HA	2.01	0.42
1:B:78:ALA:N	1:B:79:PRO:HD2	2.34	0.42
1:B:141:THR:HG23	4:B:404:HOH:O	2.19	0.42
1:B:229:THR:HB	1:B:230:PRO:CD	2.49	0.42
1:C:225:PHE:CE2	1:C:246:VAL:CG1	3.02	0.42
1:C:347:TYR:CD1	1:C:352:VAL:HB	2.55	0.42
1:E:47:VAL:HG11	1:E:121:SER:OG	2.19	0.42
1:E:92:ILE:O	1:E:96:LEU:HG	2.20	0.42
1:G:93:MSE:HE1	1:G:96:LEU:HD11	2.02	0.42
1:A:341:ILE:O	1:A:342:VAL:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ILE:HD11	1:D:86:VAL:HA	2.02	0.42
1:E:45:ASN:HD22	1:E:46:GLY:N	2.18	0.42
1:G:89:LEU:HD13	1:G:114:MSE:HB2	2.01	0.42
1:C:108:ALA:HB2	1:C:280:GLY:HA2	2.02	0.42
1:D:249:MSE:HA	1:D:271:VAL:O	2.20	0.42
1:D:306:GLU:HB3	1:D:310:GLY:HA3	2.01	0.42
1:E:244:THR:OG1	1:E:246:VAL:CG1	2.68	0.42
1:G:15:ILE:HG12	1:G:66:VAL:HG22	2.01	0.42
1:G:141:THR:HG21	1:G:198:ARG:NH1	2.34	0.42
1:G:359:GLY:C	1:G:361:GLY:H	2.28	0.42
1:A:89:LEU:C	1:A:89:LEU:HD12	2.45	0.42
1:A:341:ILE:O	1:A:363:ASP:O	2.38	0.42
1:C:45:ASN:HD22	1:C:45:ASN:N	2.16	0.42
1:C:111:ASP:O	1:C:115:HIS:HD2	2.02	0.42
1:C:275:LYS:HB2	1:C:278:LYS:HB3	2.01	0.42
1:E:214:LEU:N	1:E:215:PRO:CD	2.83	0.42
1:F:8:ILE:HD11	1:F:86:VAL:CA	2.49	0.42
1:G:315:LEU:HD13	1:G:355:PRO:HD3	2.02	0.42
1:H:238:ARG:HE	1:H:242:ARG:NH1	2.18	0.42
1:C:43:LEU:HD12	1:C:47:VAL:HG13	2.02	0.41
1:C:191:VAL:O	1:C:193:ASP:N	2.53	0.41
1:E:18:VAL:HA	1:E:19:PRO:HD3	1.84	0.41
1:G:127:ARG:N	1:G:316:GLN:HE21	2.12	0.41
1:B:11:VAL:HG11	1:B:81:LEU:HD22	2.01	0.41
1:D:89:LEU:C	1:D:89:LEU:HD12	2.45	0.41
1:D:274:LEU:C	1:D:274:LEU:HD12	2.46	0.41
1:F:207:ARG:HB3	1:H:296:GLY:O	2.21	0.41
1:G:43:LEU:HD12	1:G:47:VAL:HG11	2.01	0.41
1:B:92:ILE:CD1	1:B:114:MSE:HE1	2.50	0.41
1:B:115:HIS:HE1	4:B:434:HOH:O	2.03	0.41
1:C:331:PHE:CD1	1:C:331:PHE:C	2.98	0.41
1:C:341:ILE:HG13	1:C:341:ILE:O	2.20	0.41
1:D:8:ILE:HG12	1:D:114:MSE:HE3	2.01	0.41
1:D:92:ILE:HG22	1:D:93:MSE:HE2	2.02	0.41
1:E:269:ALA:O	1:E:297:LEU:HD22	2.20	0.41
1:F:135:ARG:HD2	1:F:138:VAL:CG1	2.49	0.41
1:G:89:LEU:O	1:G:93:MSE:HG2	2.21	0.41
1:A:149:LEU:O	1:A:153:VAL:HG23	2.20	0.41
1:C:8:ILE:HD11	1:C:86:VAL:HA	2.03	0.41
1:C:342:VAL:HB	1:C:343:GLN:OE1	2.20	0.41
1:D:311:THR:OG1	1:D:333:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:GLY:O	1:G:207:ARG:HB3	2.20	0.41
1:F:11:VAL:HG12	1:F:41:VAL:HG22	2.03	0.41
1:F:146:VAL:O	1:F:147:LEU:HD23	2.21	0.41
1:A:341:ILE:O	1:A:341:ILE:HG23	2.20	0.41
1:D:18:VAL:HA	1:D:19:PRO:HD3	1.83	0.41
1:D:225:PHE:CE2	1:D:246:VAL:CG1	3.03	0.41
1:E:52:GLU:CD	1:E:310:GLY:H	2.29	0.41
1:E:169:LYS:HE3	1:E:200:ASP:HB2	2.03	0.41
1:H:341:ILE:O	1:H:342:VAL:CB	2.65	0.41
1:B:279:HIS:CG	1:B:288:ILE:HG13	2.55	0.41
1:D:34:GLN:HE21	1:D:305:LEU:HB3	1.84	0.41
1:E:211:LEU:CD2	1:E:240:ILE:HG22	2.51	0.41
1:E:331:PHE:CD1	1:E:331:PHE:C	2.99	0.41
1:H:69:MSE:O	1:H:73:VAL:HG23	2.20	0.41
1:B:8:ILE:HG21	1:B:81:LEU:HB3	2.01	0.41
1:C:244:THR:O	1:C:245:ASN:HB2	2.20	0.41
1:D:92:ILE:CD1	1:D:114:MSE:HE1	2.50	0.41
1:G:176:ASP:HA	1:G:177:PRO:HD3	1.93	0.41
1:G:244:THR:OG1	1:G:246:VAL:HG13	2.21	0.41
1:A:43:LEU:HB2	1:A:45:ASN:ND2	2.33	0.41
1:B:302:ALA:HA	1:B:329:GLU:HG2	2.02	0.41
1:B:347:TYR:O	1:B:348:LYS:HB3	2.20	0.41
1:D:11:VAL:HG23	1:D:78:ALA:HB1	2.01	0.41
1:D:104:ARG:O	1:D:280:GLY:HA2	2.20	0.41
1:D:360:LEU:HD12	1:D:360:LEU:HA	1.89	0.41
1:E:56:PRO:HG3	1:E:304:SER:HA	2.02	0.41
1:F:18:VAL:HA	1:F:19:PRO:HD3	1.85	0.41
1:F:289:ALA:HB1	1:F:323:ALA:HB3	2.03	0.41
1:A:125:PRO:HB2	1:A:127:ARG:HG2	2.03	0.41
1:A:226:GLU:O	1:A:227:GLN:C	2.63	0.41
1:C:347:TYR:CE1	1:C:352:VAL:HB	2.55	0.41
1:D:309:ILE:HD11	1:D:341:ILE:HD11	2.03	0.41
1:F:25:GLY:CA	1:F:146:VAL:HG12	2.51	0.41
1:H:93:MSE:HA	1:H:93:MSE:HE2	2.02	0.41
1:H:201:ILE:HD12	1:H:228:PRO:CB	2.50	0.41
1:A:346:GLU:O	1:A:352:VAL:HA	2.21	0.41
1:C:341:ILE:HG12	1:C:362:VAL:HG13	2.03	0.41
1:D:225:PHE:CE2	1:D:246:VAL:HG11	2.56	0.41
1:D:341:ILE:O	1:D:363:ASP:O	2.39	0.41
1:E:341:ILE:O	1:E:343:GLN:N	2.51	0.41
1:H:187:LEU:HD23	1:H:187:LEU:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:8:ILE:HD11	1:G:86:VAL:CB	2.51	0.40
1:G:313:ALA:HA	1:G:360:LEU:CD1	2.51	0.40
1:H:341:ILE:HG12	1:H:362:VAL:CG2	2.51	0.40
1:B:18:VAL:HA	1:B:19:PRO:HD3	1.86	0.40
1:B:87:SER:HA	1:B:118:TRP:CZ2	2.57	0.40
1:F:238:ARG:HG3	1:F:242:ARG:CZ	2.51	0.40
1:G:50:TYR:CZ	1:G:364:VAL:HG21	2.56	0.40
1:G:343:GLN:NE2	1:G:363:ASP:OD1	2.54	0.40
1:A:88:GLU:O	1:A:89:LEU:C	2.64	0.40
1:A:185:ALA:O	1:A:189:ARG:NH1	2.55	0.40
1:E:240:ILE:HD11	1:E:248:VAL:CG2	2.51	0.40
1:H:275:LYS:HB2	1:H:278:LYS:HB3	2.03	0.40
1:E:127:ARG:HH11	1:E:316:GLN:HE22	1.70	0.40
1:F:275:LYS:HB2	1:F:278:LYS:HB3	2.04	0.40
1:F:308:PRO:HD2	1:F:340:TYR:CE1	2.57	0.40
1:G:346:GLU:O	1:G:352:VAL:HA	2.21	0.40
1:C:22:ARG:HG2	1:C:22:ARG:HH11	1.87	0.40
1:D:238:ARG:NH2	1:H:242:ARG:HH21	2.19	0.40
1:D:341:ILE:O	1:D:342:VAL:HB	2.21	0.40
1:G:127:ARG:HG2	1:G:316:GLN:HE22	1.87	0.40

There are no symmetry-related clashes.

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	368/383 (96%)	350 (95%)	18 (5%)	0	100	100
1	B	368/383 (96%)	349 (95%)	19 (5%)	0	100	100
1	C	368/383 (96%)	344 (94%)	22 (6%)	2 (0%)	24	27
1	D	368/383 (96%)	346 (94%)	22 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	368/383 (96%)	350 (95%)	18 (5%)	0	100	100
1	F	368/383 (96%)	344 (94%)	24 (6%)	0	100	100
1	G	368/383 (96%)	340 (92%)	27 (7%)	1 (0%)	36	42
1	H	368/383 (96%)	343 (93%)	23 (6%)	2 (0%)	24	27
All	All	2944/3064 (96%)	2766 (94%)	173 (6%)	5 (0%)	43	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	192	GLY
1	H	192	GLY
1	G	332	GLY
1	H	342	VAL
1	C	342	VAL

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	291/296 (98%)	279 (96%)	12 (4%)	27	37
1	B	291/296 (98%)	277 (95%)	14 (5%)	23	30
1	C	291/296 (98%)	274 (94%)	17 (6%)	18	22
1	D	291/296 (98%)	279 (96%)	12 (4%)	27	37
1	E	291/296 (98%)	275 (94%)	16 (6%)	19	24
1	F	291/296 (98%)	274 (94%)	17 (6%)	18	22
1	G	291/296 (98%)	281 (97%)	10 (3%)	32	44
1	H	291/296 (98%)	279 (96%)	12 (4%)	27	37
All	All	2328/2368 (98%)	2218 (95%)	110 (5%)	23	31

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	68	THR
1	A	89	LEU
1	A	240	ILE
1	A	246	VAL
1	A	252	GLU
1	A	261	LEU
1	A	274	LEU
1	A	305	LEU
1	A	341	ILE
1	A	360	LEU
1	A	363	ASP
1	B	6	LEU
1	B	45	ASN
1	B	89	LEU
1	B	133	THR
1	B	161	GLU
1	B	240	ILE
1	B	246	VAL
1	B	252	GLU
1	B	261	LEU
1	B	274	LEU
1	B	305	LEU
1	B	322	LYS
1	B	335	LEU
1	B	341	ILE
1	C	6	LEU
1	C	11	VAL
1	C	45	ASN
1	C	68	THR
1	C	111	ASP
1	C	133	THR
1	C	135	ARG
1	C	141	THR
1	C	240	ILE
1	C	246	VAL
1	C	252	GLU
1	C	261	LEU
1	C	274	LEU
1	C	305	LEU
1	C	322	LYS
1	C	335	LEU
1	C	360	LEU

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Mol	Chain	Res	Type
1	D	6	LEU
1	D	18	VAL
1	D	45	ASN
1	D	89	LEU
1	D	133	THR
1	D	246	VAL
1	D	252	GLU
1	D	261	LEU
1	D	274	LEU
1	D	305	LEU
1	D	322	LYS
1	D	360	LEU
1	E	6	LEU
1	E	18	VAL
1	E	45	ASN
1	E	68	THR
1	E	89	LEU
1	E	111	ASP
1	E	133	THR
1	E	161	GLU
1	E	182	ARG
1	E	246	VAL
1	E	252	GLU
1	E	261	LEU
1	E	274	LEU
1	E	305	LEU
1	E	322	LYS
1	E	360	LEU
1	F	45	ASN
1	F	54	VAL
1	F	68	THR
1	F	133	THR
1	F	182	ARG
1	F	240	ILE
1	F	246	VAL
1	F	252	GLU
1	F	257	PRO
1	F	261	LEU
1	F	274	LEU
1	F	305	LEU
1	F	322	LYS
1	F	335	LEU

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Mol	Chain	Res	Type
1	F	341	ILE
1	F	360	LEU
1	F	362	VAL
1	G	45	ASN
1	G	133	THR
1	G	182	ARG
1	G	246	VAL
1	G	252	GLU
1	G	261	LEU
1	G	274	LEU
1	G	305	LEU
1	G	322	LYS
1	G	360	LEU
1	H	45	ASN
1	H	133	THR
1	H	161	GLU
1	H	240	ILE
1	H	246	VAL
1	H	252	GLU
1	H	261	LEU
1	H	274	LEU
1	H	305	LEU
1	H	322	LYS
1	H	360	LEU
1	H	362	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	45	ASN
1	A	115	HIS
1	A	202	ASN
1	A	212	HIS
1	A	316	GLN
1	A	351	GLN
1	A	370	ASN
1	B	45	ASN
1	B	115	HIS
1	B	212	HIS
1	B	245	ASN
1	B	316	GLN

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Mol	Chain	Res	Type
1	B	370	ASN
1	C	45	ASN
1	C	115	HIS
1	C	212	HIS
1	C	316	GLN
1	C	351	GLN
1	C	370	ASN
1	D	45	ASN
1	D	245	ASN
1	D	316	GLN
1	D	370	ASN
1	E	9	GLN
1	E	45	ASN
1	E	115	HIS
1	E	202	ASN
1	E	316	GLN
1	E	370	ASN
1	F	42	HIS
1	F	45	ASN
1	F	115	HIS
1	F	316	GLN
1	F	370	ASN
1	G	45	ASN
1	G	115	HIS
1	G	165	ASN
1	G	202	ASN
1	G	245	ASN
1	G	316	GLN
1	G	351	GLN
1	G	370	ASN
1	H	9	GLN
1	H	45	ASN
1	H	115	HIS
1	H	316	GLN
1	H	370	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACY	D	384	3	3,3,3	0.81	0	3,3,3	0.85	0
2	ACY	A	384	3	3,3,3	0.47	0	3,3,3	0.69	0
2	ACY	H	384	3	3,3,3	0.69	0	3,3,3	1.00	0
2	ACY	G	384	3	3,3,3	0.75	0	3,3,3	0.76	0
2	ACY	B	384	3	3,3,3	0.58	0	3,3,3	0.90	0
2	ACY	F	384	3	3,3,3	0.57	0	3,3,3	0.82	0
2	ACY	C	384	3	3,3,3	0.52	0	3,3,3	0.95	0
2	ACY	E	384	3	3,3,3	0.67	0	3,3,3	0.88	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	364/383 (95%)	0.32	11 (3%) 52 49	26, 44, 64, 71	0
1	B	364/383 (95%)	0.27	8 (2%) 62 59	25, 43, 65, 77	0
1	C	364/383 (95%)	0.33	11 (3%) 52 49	25, 46, 70, 80	0
1	D	364/383 (95%)	0.40	25 (6%) 23 20	27, 45, 74, 86	0
1	E	364/383 (95%)	0.16	8 (2%) 62 59	23, 40, 61, 71	0
1	F	364/383 (95%)	0.39	18 (4%) 35 31	27, 45, 69, 80	0
1	G	364/383 (95%)	0.87	35 (9%) 13 11	30, 54, 79, 87	0
1	H	364/383 (95%)	0.59	26 (7%) 22 19	28, 48, 73, 85	0
All	All	2912/3064 (95%)	0.42	142 (4%) 35 31	23, 45, 72, 87	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	341	ILE	4.7
1	H	152	ALA	4.5
1	D	341	ILE	4.4
1	F	341	ILE	4.3
1	B	341	ILE	4.2
1	A	341	ILE	4.0
1	F	146	VAL	3.8
1	E	341	ILE	3.8
1	H	11	VAL	3.7
1	H	26	PHE	3.6
1	C	341	ILE	3.5
1	H	145	GLY	3.4
1	G	156	ILE	3.4
1	A	18	VAL	3.3
1	D	153	VAL	3.3
1	A	9	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	50	TYR	3.3
1	G	364	VAL	3.3
1	C	18	VAL	3.2
1	E	342	VAL	3.2
1	D	191	VAL	3.1
1	D	152	ALA	3.1
1	D	151	VAL	3.1
1	H	146	VAL	3.1
1	G	151	VAL	3.1
1	H	192	GLY	3.1
1	G	47	VAL	3.1
1	H	341	ILE	3.0
1	G	16	LEU	3.0
1	G	18	VAL	3.0
1	H	27	ALA	2.9
1	G	191	VAL	2.9
1	G	11	VAL	2.9
1	E	240	ILE	2.9
1	A	11	VAL	2.9
1	H	151	VAL	2.9
1	G	6	LEU	2.8
1	G	43	LEU	2.8
1	A	6	LEU	2.8
1	C	152	ALA	2.8
1	D	18	VAL	2.8
1	G	340	TYR	2.7
1	D	146	VAL	2.7
1	F	145	GLY	2.7
1	G	373	THR	2.7
1	D	25	GLY	2.7
1	D	160	ILE	2.7
1	G	357	GLY	2.7
1	G	44	GLU	2.7
1	H	190	GLU	2.7
1	D	149	LEU	2.7
1	G	168	PHE	2.7
1	A	21	ILE	2.6
1	E	44	GLU	2.6
1	G	347	TYR	2.6
1	H	5	ASP	2.6
1	E	191	VAL	2.6
1	C	192	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	154	ALA	2.6
1	D	156	ILE	2.6
1	A	5	ASP	2.5
1	H	49	GLY	2.5
1	H	148	PRO	2.5
1	F	18	VAL	2.5
1	F	152	ALA	2.5
1	D	148	PRO	2.5
1	H	6	LEU	2.5
1	G	25	GLY	2.5
1	B	11	VAL	2.4
1	H	153	VAL	2.4
1	H	144	LEU	2.4
1	G	23	PRO	2.4
1	B	191	VAL	2.4
1	G	342	VAL	2.4
1	H	118	TRP	2.4
1	G	335	LEU	2.4
1	F	339	THR	2.4
1	D	362	VAL	2.4
1	E	18	VAL	2.4
1	H	8	ILE	2.4
1	E	340	TYR	2.4
1	G	5	ASP	2.4
1	G	339	THR	2.4
1	H	364	VAL	2.4
1	D	9	GLN	2.4
1	F	337	LYS	2.3
1	C	342	VAL	2.3
1	D	163	PHE	2.3
1	F	342	VAL	2.3
1	G	362	VAL	2.3
1	H	147	LEU	2.3
1	D	145	GLY	2.3
1	G	356	GLN	2.3
1	B	364	VAL	2.3
1	F	5	ASP	2.3
1	B	9	GLN	2.3
1	C	151	VAL	2.3
1	D	26	PHE	2.2
1	G	352	VAL	2.3
1	H	124	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	6	LEU	2.2
1	G	144	LEU	2.2
1	H	47	VAL	2.2
1	E	5	ASP	2.2
1	A	44	GLU	2.2
1	D	24	HIS	2.2
1	D	157	GLU	2.2
1	G	160	ILE	2.2
1	D	342	VAL	2.2
1	D	150	ASP	2.2
1	G	178	ALA	2.2
1	H	340	TYR	2.2
1	D	240	ILE	2.2
1	F	149	LEU	2.2
1	A	191	VAL	2.2
1	H	346	GLU	2.2
1	F	27	ALA	2.2
1	A	340	TYR	2.1
1	B	340	TYR	2.1
1	C	8	ILE	2.1
1	F	147	LEU	2.1
1	G	48	ILE	2.1
1	B	18	VAL	2.1
1	A	22	ARG	2.1
1	G	15	ILE	2.1
1	G	309	ILE	2.1
1	C	5	ASP	2.1
1	G	157	GLU	2.1
1	F	47	VAL	2.1
1	D	29	THR	2.1
1	C	150	ASP	2.1
1	B	47	VAL	2.1
1	F	26	PHE	2.1
1	D	147	LEU	2.1
1	F	240	ILE	2.1
1	C	340	TYR	2.1
1	F	192	GLY	2.1
1	D	5	ASP	2.0
1	H	156	ILE	2.0
1	F	340	TYR	2.0
1	C	191	VAL	2.0
1	G	336	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACY	D	384	4/4	0.86	0.14	44,45,46,46	0
2	ACY	G	384	4/4	0.88	0.12	48,49,49,50	0
2	ACY	B	384	4/4	0.91	0.09	28,28,29,29	0
2	ACY	F	384	4/4	0.92	0.12	39,39,40,40	0
2	ACY	C	384	4/4	0.94	0.09	40,40,40,41	0
2	ACY	E	384	4/4	0.94	0.07	31,31,32,32	0
2	ACY	H	384	4/4	0.94	0.10	41,42,45,45	0
2	ACY	A	384	4/4	0.95	0.09	32,34,34,34	0
3	MG	A	385	1/1	0.97	0.09	28,28,28,28	0
3	MG	C	385	1/1	0.97	0.05	31,31,31,31	0
3	MG	D	385	1/1	0.97	0.07	33,33,33,33	0
3	MG	E	385	1/1	0.98	0.03	24,24,24,24	0
3	MG	F	385	1/1	0.98	0.06	31,31,31,31	0
3	MG	G	385	1/1	0.98	0.08	38,38,38,38	0
3	MG	H	385	1/1	0.98	0.07	35,35,35,35	0
3	MG	B	385	1/1	0.99	0.03	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.