



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:12 AM UTC

PDB ID : 3NO1 / pdb_00003no1
Title : Crystal Structure of Mandelate racemase/muconate lactonizing enzyme from a Marine actinobacterium in complex with magnesium
Authors : Satyanarayana, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-06-24
Resolution : 2.16 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

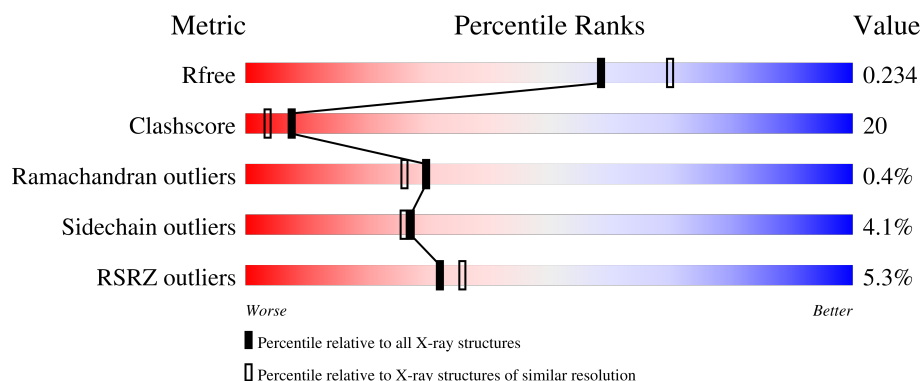
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	398	3% 63% 24% • 11%
1	B	398	5% 56% 27% • 12%
1	C	398	3% 63% 25% • 10%
1	D	398	5% 55% 31% • 12%
1	E	398	5% 54% 29% 5% 11%

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Mol	Chain	Length	Quality of chain
1	F	398	6% 55% 28% 5% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17170 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 Mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	Se	0	0	0
			2782	1757	488	522	5	10			
1	B	349	Total	C	N	O	S	Se	0	0	0
			2734	1726	477	516	5	10			
1	C	357	Total	C	N	O	S	Se	0	0	0
			2792	1762	490	525	5	10			
1	D	350	Total	C	N	O	S	Se	0	0	0
			2745	1732	481	517	5	10			
1	E	353	Total	C	N	O	S	Se	0	0	0
			2762	1742	484	521	5	10			
1	F	349	Total	C	N	O	S	Se	0	0	0
			2723	1718	476	514	5	10			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP A4AFX2
A	0	SER	-	expression tag	UNP A4AFX2
A	1	LEU	-	expression tag	UNP A4AFX2
A	389	GLU	-	expression tag	UNP A4AFX2
A	390	GLY	-	expression tag	UNP A4AFX2
A	391	HIS	-	expression tag	UNP A4AFX2
A	392	HIS	-	expression tag	UNP A4AFX2
A	393	HIS	-	expression tag	UNP A4AFX2
A	394	HIS	-	expression tag	UNP A4AFX2
A	395	HIS	-	expression tag	UNP A4AFX2
A	396	HIS	-	expression tag	UNP A4AFX2
B	-1	MSE	-	expression tag	UNP A4AFX2
B	0	SER	-	expression tag	UNP A4AFX2
B	1	LEU	-	expression tag	UNP A4AFX2
B	389	GLU	-	expression tag	UNP A4AFX2
B	390	GLY	-	expression tag	UNP A4AFX2
B	391	HIS	-	expression tag	UNP A4AFX2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	392	HIS	-	expression tag	UNP A4AFX2
B	393	HIS	-	expression tag	UNP A4AFX2
B	394	HIS	-	expression tag	UNP A4AFX2
B	395	HIS	-	expression tag	UNP A4AFX2
B	396	HIS	-	expression tag	UNP A4AFX2
C	-1	MSE	-	expression tag	UNP A4AFX2
C	0	SER	-	expression tag	UNP A4AFX2
C	1	LEU	-	expression tag	UNP A4AFX2
C	389	GLU	-	expression tag	UNP A4AFX2
C	390	GLY	-	expression tag	UNP A4AFX2
C	391	HIS	-	expression tag	UNP A4AFX2
C	392	HIS	-	expression tag	UNP A4AFX2
C	393	HIS	-	expression tag	UNP A4AFX2
C	394	HIS	-	expression tag	UNP A4AFX2
C	395	HIS	-	expression tag	UNP A4AFX2
C	396	HIS	-	expression tag	UNP A4AFX2
D	-1	MSE	-	expression tag	UNP A4AFX2
D	0	SER	-	expression tag	UNP A4AFX2
D	1	LEU	-	expression tag	UNP A4AFX2
D	389	GLU	-	expression tag	UNP A4AFX2
D	390	GLY	-	expression tag	UNP A4AFX2
D	391	HIS	-	expression tag	UNP A4AFX2
D	392	HIS	-	expression tag	UNP A4AFX2
D	393	HIS	-	expression tag	UNP A4AFX2
D	394	HIS	-	expression tag	UNP A4AFX2
D	395	HIS	-	expression tag	UNP A4AFX2
D	396	HIS	-	expression tag	UNP A4AFX2
E	-1	MSE	-	expression tag	UNP A4AFX2
E	0	SER	-	expression tag	UNP A4AFX2
E	1	LEU	-	expression tag	UNP A4AFX2
E	389	GLU	-	expression tag	UNP A4AFX2
E	390	GLY	-	expression tag	UNP A4AFX2
E	391	HIS	-	expression tag	UNP A4AFX2
E	392	HIS	-	expression tag	UNP A4AFX2
E	393	HIS	-	expression tag	UNP A4AFX2
E	394	HIS	-	expression tag	UNP A4AFX2
E	395	HIS	-	expression tag	UNP A4AFX2
E	396	HIS	-	expression tag	UNP A4AFX2
F	-1	MSE	-	expression tag	UNP A4AFX2
F	0	SER	-	expression tag	UNP A4AFX2
F	1	LEU	-	expression tag	UNP A4AFX2
F	389	GLU	-	expression tag	UNP A4AFX2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	390	GLY	-	expression tag	UNP A4AFX2
F	391	HIS	-	expression tag	UNP A4AFX2
F	392	HIS	-	expression tag	UNP A4AFX2
F	393	HIS	-	expression tag	UNP A4AFX2
F	394	HIS	-	expression tag	UNP A4AFX2
F	395	HIS	-	expression tag	UNP A4AFX2
F	396	HIS	-	expression tag	UNP A4AFX2

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

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

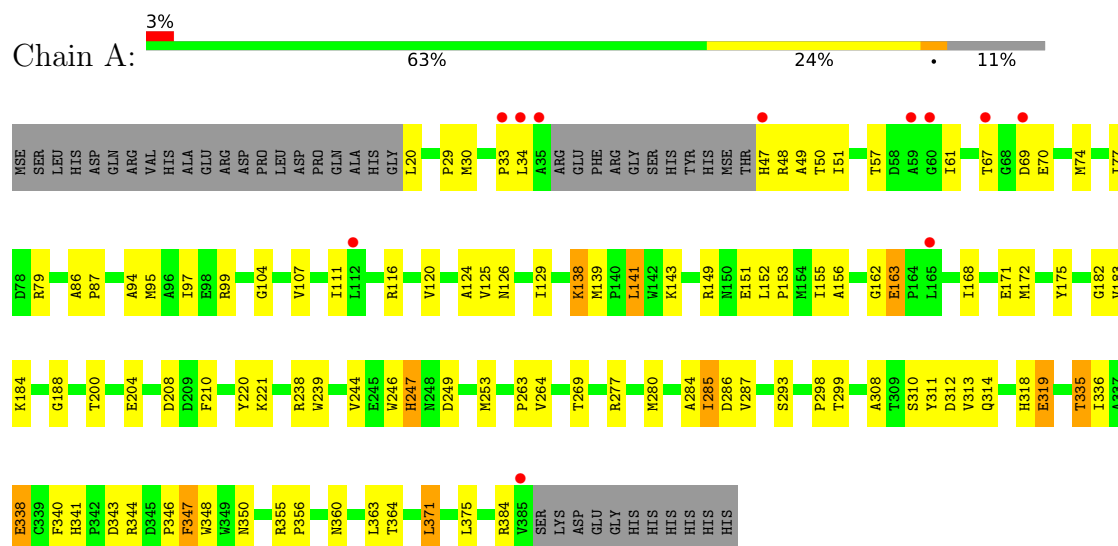
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	137	Total 137	O 137	0	0
3	B	84	Total 84	O 84	0	0
3	C	136	Total 136	O 136	0	0
3	D	88	Total 88	O 88	0	0
3	E	80	Total 80	O 80	0	0
3	F	101	Total 101	O 101	0	0

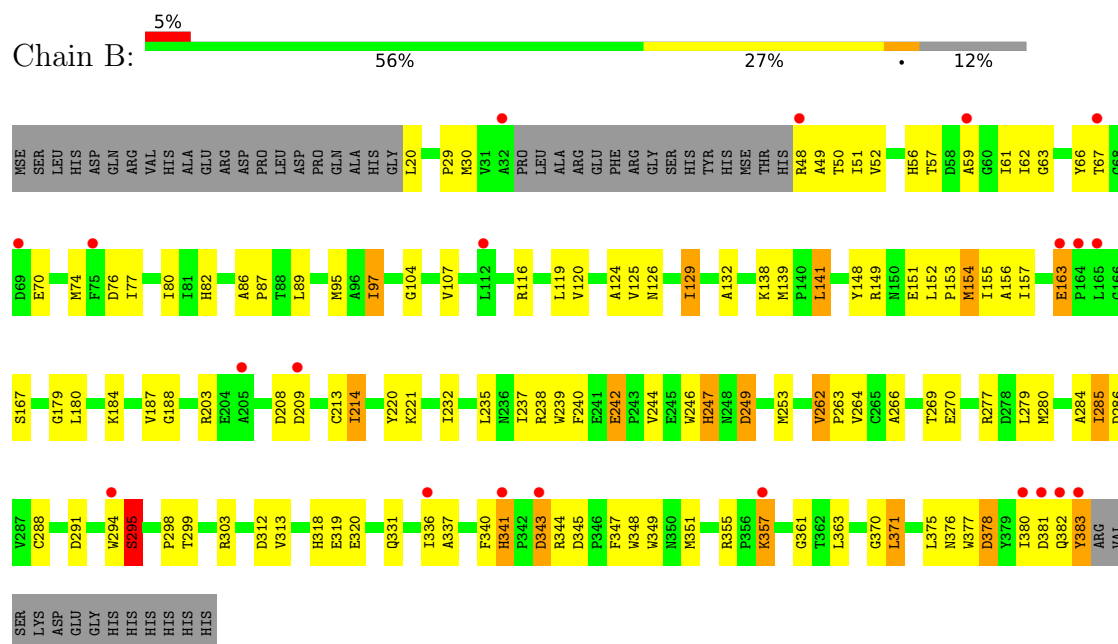
3 Residue-property plots [i](#)

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: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- Chain C:

- [illegible]

- Chain E:
-

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.96Å 90.10Å 94.66Å 115.80° 109.75° 97.58°	Depositor
Resolution (Å)	42.51 – 2.16 42.51 – 2.16	Depositor EDS
% Data completeness (in resolution range)	96.0 (42.51-2.16) 96.1 (42.51-2.16)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.97 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.240 0.202 , 0.234	Depositor DCC
R_{free} test set	4670 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17170	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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

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	0/2841	0.96	12/3851 (0.3%)
1	B	0.41	0/2791	0.98	17/3782 (0.4%)
1	C	0.43	0/2851	0.97	14/3864 (0.4%)
1	D	0.41	0/2802	0.97	13/3796 (0.3%)
1	E	0.40	0/2819	0.98	16/3819 (0.4%)
1	F	0.44	0/2779	1.01	17/3765 (0.5%)
All	All	0.42	0/16883	0.98	89/22877 (0.4%)

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	246	TRP	N-CA-C	11.72	123.61	111.07
1	F	246	TRP	N-CA-C	11.54	123.86	111.28
1	E	246	TRP	N-CA-C	11.05	122.89	111.07
1	A	246	TRP	N-CA-C	11.04	122.88	111.07
1	B	246	TRP	N-CA-C	10.85	122.68	111.07
1	D	295	SER	N-CA-C	10.00	122.44	110.44
1	C	246	TRP	N-CA-C	9.46	121.59	111.28
1	C	221	LYS	N-CA-C	-9.19	97.60	110.29
1	B	286	ASP	N-CA-C	-8.85	102.61	113.41
1	B	244	VAL	N-CA-C	8.68	121.29	108.96
1	A	221	LYS	N-CA-C	-8.39	98.71	110.29
1	B	221	LYS	N-CA-C	-8.29	99.62	110.39
1	D	61	ILE	N-CA-C	8.26	120.51	109.37
1	E	286	ASP	N-CA-C	-8.09	103.54	113.41
1	C	244	VAL	N-CA-C	7.93	120.22	108.96
1	F	286	ASP	N-CA-C	-7.92	104.13	113.88
1	F	221	LYS	N-CA-C	-7.87	99.43	110.29
1	C	347	PHE	N-CA-C	7.80	119.56	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	221	LYS	N-CA-C	-7.75	98.93	110.24
1	B	295	SER	N-CA-C	7.58	120.91	110.06
1	C	208	ASP	N-CA-C	7.58	119.62	111.36
1	E	295	SER	N-CA-C	7.58	120.89	110.06
1	F	244	VAL	N-CA-C	7.45	119.54	108.96
1	A	244	VAL	N-CA-C	7.39	119.46	108.96
1	D	221	LYS	N-CA-C	-7.39	99.45	110.24
1	E	244	VAL	N-CA-C	7.34	119.39	108.96
1	F	219	GLY	N-CA-C	7.34	123.76	114.66
1	E	242	GLU	CB-CA-C	-7.32	106.00	111.20
1	E	247	HIS	N-CA-C	7.20	119.75	111.11
1	E	249	ASP	N-CA-C	7.14	119.07	111.28
1	B	285	ILE	N-CA-C	7.07	120.38	108.86
1	A	347	PHE	N-CA-C	7.02	118.82	111.03
1	A	247	HIS	N-CA-C	6.95	119.45	111.11
1	F	295	SER	N-CA-C	6.94	119.28	110.61
1	E	208	ASP	N-CA-C	6.87	118.42	111.07
1	C	286	ASP	N-CA-C	-6.85	105.05	113.41
1	A	286	ASP	N-CA-C	-6.77	105.15	113.41
1	B	97	ILE	N-CA-C	6.76	117.45	110.36
1	B	61	ILE	N-CA-C	6.74	117.72	109.30
1	D	286	ASP	N-CA-C	-6.73	105.19	113.41
1	D	244	VAL	N-CA-C	6.70	119.44	108.99
1	D	285	ILE	N-CA-C	6.67	119.61	108.81
1	F	285	ILE	N-CA-C	6.58	119.80	108.95
1	A	285	ILE	N-CA-C	6.52	119.73	108.90
1	C	247	HIS	N-CA-C	6.40	118.79	111.11
1	D	59	ALA	N-CA-C	-6.35	100.51	110.36
1	A	249	ASP	N-CA-C	6.34	119.00	111.33
1	E	285	ILE	N-CA-C	6.33	119.17	108.86
1	B	208	ASP	N-CA-C	6.25	117.89	111.14
1	F	380	ILE	N-CA-C	6.18	117.27	108.93
1	A	335	THR	N-CA-C	6.16	118.64	108.48
1	C	249	ASP	N-CA-C	6.05	117.88	111.28
1	F	254	ARG	N-CA-C	-6.02	104.72	111.28
1	F	247	HIS	N-CA-C	5.97	118.28	111.11
1	E	256	VAL	N-CA-C	-5.93	104.73	110.72
1	C	295	SER	N-CA-C	5.90	119.70	111.56
1	B	59	ALA	N-CA-C	-5.89	102.05	110.59
1	B	247	HIS	N-CA-C	5.87	118.16	111.11
1	B	331	GLN	N-CA-C	5.87	118.41	110.31
1	C	285	ILE	N-CA-C	5.87	118.64	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	347	PHE	N-CA-C	5.82	117.32	110.97
1	C	112	LEU	N-CA-C	5.81	119.99	113.02
1	A	61	ILE	N-CA-C	5.79	116.82	108.48
1	F	297	GLY	CA-C-N	5.75	125.87	119.32
1	F	297	GLY	C-N-CA	5.75	125.87	119.32
1	F	249	ASP	N-CA-C	5.73	118.27	111.33
1	C	351	MSE	N-CA-C	5.72	117.52	111.28
1	B	82	HIS	N-CA-C	5.67	117.54	111.36
1	B	242	GLU	CB-CA-C	-5.62	107.21	111.20
1	B	378	ASP	N-CA-C	-5.55	104.86	111.69
1	A	208	ASP	N-CA-C	5.54	118.25	111.82
1	D	331	GLN	N-CA-C	5.53	117.94	110.31
1	D	249	ASP	N-CA-C	5.53	117.31	111.28
1	A	97	ILE	N-CA-C	5.52	116.91	110.62
1	D	247	HIS	N-CA-C	5.49	117.97	111.33
1	F	97	ILE	N-CA-C	5.48	116.21	110.62
1	F	140	PRO	N-CA-C	-5.48	102.59	111.19
1	E	254	ARG	N-CA-C	-5.47	105.39	111.36
1	D	97	ILE	N-CA-C	5.41	116.79	110.62
1	B	249	ASP	N-CA-C	5.39	117.58	111.11
1	F	335	THR	N-CA-C	5.39	117.38	108.48
1	E	331	GLN	N-CA-C	5.28	117.60	110.31
1	F	137	LEU	N-CA-C	5.26	119.55	113.18
1	C	331	GLN	N-CA-C	5.22	116.65	110.07
1	E	61	ILE	N-CA-C	5.22	116.49	108.71
1	D	351	MSE	N-CA-C	5.20	119.68	113.23
1	C	335	THR	N-CA-C	5.13	116.94	108.48
1	E	141	LEU	N-CA-C	5.07	116.81	111.28
1	B	341	HIS	N-CA-C	-5.05	103.42	109.83

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	2782	0	2685	108	0
1	B	2734	0	2632	130	0
1	C	2792	0	2692	85	0
1	D	2745	0	2645	110	0
1	E	2762	0	2662	130	0
1	F	2723	0	2622	120	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
3	A	137	0	0	5	0
3	B	84	0	0	8	0
3	C	136	0	0	5	0
3	D	88	0	0	8	0
3	E	80	0	0	4	0
3	F	101	0	0	3	0
All	All	17170	0	15938	656	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 20.

All (656) 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:A:253:MSE:HE3	1:A:264:VAL:HG12	1.32	1.07
1:F:30:MSE:HE1	1:F:380:ILE:HG23	1.34	1.05
1:A:253:MSE:HE3	1:A:264:VAL:CG1	1.86	1.05
1:A:280:MSE:HE2	1:A:311:TYR:HB2	1.40	1.04
1:F:253:MSE:HE3	1:F:264:VAL:CG1	1.90	1.01
1:E:168:ILE:HD12	1:E:168:ILE:H	1.23	1.00
1:A:280:MSE:HE3	1:A:313:VAL:HB	1.42	0.99
1:A:280:MSE:CE	1:A:308:ALA:HA	1.94	0.98
1:A:280:MSE:HE1	1:A:308:ALA:HA	1.03	0.98
1:E:95:MSE:HE2	1:E:133:VAL:HG22	1.48	0.95
1:E:153:PRO:HG2	1:E:336:ILE:HG22	1.49	0.95
1:F:253:MSE:HE3	1:F:264:VAL:HG12	1.47	0.94
1:E:250:LYS:HG2	1:E:279:LEU:HD12	1.51	0.92
1:F:253:MSE:CE	1:F:285:ILE:HG22	2.01	0.90
1:B:253:MSE:HE3	1:B:264:VAL:CG1	2.02	0.90
1:B:341:HIS:HD1	1:B:343:ASP:H	1.18	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:MSE:H	1:F:74:MSE:HE1	1.37	0.88
1:B:253:MSE:HE1	1:B:285:ILE:HG22	1.53	0.86
1:C:303:ARG:O	1:C:307:ILE:HD13	1.74	0.86
1:C:384:ARG:HD3	3:C:423:HOH:O	1.74	0.86
1:E:351:MSE:HE3	1:E:375:LEU:HD22	1.56	0.86
1:E:277:ARG:HD2	1:F:311:TYR:CE2	2.11	0.86
1:F:111:ILE:HD12	1:F:111:ILE:H	1.38	0.85
1:B:163:GLU:OE1	1:B:167:SER:HA	1.76	0.85
1:B:348:TRP:O	1:B:355:ARG:HD3	1.76	0.85
1:A:280:MSE:HE1	1:A:308:ALA:CA	1.99	0.85
1:A:253:MSE:CE	1:A:285:ILE:HG22	2.06	0.84
1:A:20:LEU:HD12	1:A:20:LEU:O	1.78	0.83
1:A:253:MSE:HE2	1:A:285:ILE:HG22	1.59	0.83
1:F:253:MSE:HE1	1:F:285:ILE:HG22	1.59	0.83
1:E:155:ILE:HD12	1:E:336:ILE:HD13	1.59	0.82
1:B:277:ARG:HG2	1:B:277:ARG:HH11	1.44	0.82
1:D:204:GLU:HG2	3:D:420:HOH:O	1.79	0.82
1:B:156:ALA:HB2	1:B:180:LEU:HD13	1.62	0.82
1:B:253:MSE:HE3	1:B:264:VAL:HG12	1.60	0.80
1:E:67:THR:HG21	1:E:124:ALA:HA	1.64	0.80
1:F:30:MSE:CE	1:F:380:ILE:HG23	2.11	0.80
1:A:280:MSE:HE3	1:A:313:VAL:CB	2.12	0.80
1:F:103:SER:O	1:F:106:LYS:HE3	1.81	0.80
1:A:280:MSE:HE2	1:A:311:TYR:CB	2.11	0.80
1:E:277:ARG:HG2	1:E:277:ARG:HH11	1.46	0.79
1:A:50:THR:O	1:A:74:MSE:HE1	1.83	0.79
1:B:125:VAL:O	1:B:129:ILE:HG23	1.83	0.79
1:F:253:MSE:HE3	1:F:264:VAL:HG11	1.66	0.78
1:D:351:MSE:HE2	1:D:375:LEU:HD22	1.66	0.78
1:A:253:MSE:CE	1:A:264:VAL:HG12	2.12	0.78
1:B:253:MSE:CE	1:B:285:ILE:HG22	2.13	0.78
1:C:50:THR:N	1:C:74:MSE:HE1	2.00	0.77
1:A:153:PRO:HG2	1:A:336:ILE:HD12	1.66	0.77
1:E:235:LEU:HB2	1:E:237:ILE:HD11	1.66	0.77
1:F:29:PRO:HA	1:F:74:MSE:HE2	1.66	0.76
1:F:142:TRP:H	1:F:326:HIS:HD2	1.34	0.76
1:D:253:MSE:CE	1:D:285:ILE:HG23	2.16	0.76
1:E:151:GLU:HG2	1:E:362:THR:HG21	1.68	0.76
1:A:280:MSE:CE	1:A:311:TYR:HB2	2.15	0.76
1:A:67:THR:HG22	3:A:432:HOH:O	1.85	0.76
1:D:376:ASN:HD21	1:D:378:ASP:HB2	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:MSE:HE2	1:E:347:PHE:HE1	1.51	0.75
1:A:311:TYR:CE2	1:B:277:ARG:HD2	2.22	0.74
1:F:126:ASN:HD22	1:F:298:PRO:HD2	1.52	0.74
1:A:139:MSE:HE1	1:B:95:MSE:HG3	1.69	0.74
1:A:344:ARG:O	1:A:344:ARG:HD3	1.87	0.74
1:F:48:ARG:HG2	1:F:347:PHE:CE2	2.21	0.74
1:F:108:THR:HG22	1:F:119:LEU:HD12	1.70	0.73
1:A:280:MSE:CE	1:A:313:VAL:HB	2.17	0.73
1:D:253:MSE:HE3	1:D:285:ILE:HG23	1.69	0.73
1:D:190:LEU:HD23	1:D:194:GLU:HG2	1.71	0.72
1:E:95:MSE:CE	1:E:133:VAL:HG22	2.19	0.72
1:D:89:LEU:HD11	1:D:125:VAL:HG11	1.71	0.72
1:E:114:ASP:HB3	1:E:117:LEU:CD2	2.19	0.72
1:B:89:LEU:HD11	1:B:125:VAL:HG11	1.71	0.72
1:D:153:PRO:HG2	1:D:336:ILE:CD1	2.20	0.71
1:C:89:LEU:HD11	1:C:125:VAL:HG11	1.72	0.71
1:B:141:LEU:HD22	1:B:370:GLY:C	2.15	0.71
1:A:253:MSE:HE2	1:A:285:ILE:CG2	2.21	0.71
1:A:153:PRO:HG2	1:A:336:ILE:CD1	2.19	0.71
1:A:247:HIS:HE1	1:F:312:ASP:OD1	1.73	0.71
1:B:235:LEU:HB2	1:B:237:ILE:HD11	1.71	0.71
1:F:253:MSE:HE2	1:F:285:ILE:HG22	1.71	0.71
1:F:253:MSE:CE	1:F:264:VAL:HG12	2.19	0.71
1:C:250:LYS:HG2	1:C:279:LEU:HD12	1.73	0.70
1:F:174:ASN:HD21	1:F:341:HIS:HE2	1.39	0.69
1:B:253:MSE:HE3	1:B:264:VAL:HG11	1.74	0.69
1:B:344:ARG:HG2	1:B:344:ARG:HH11	1.57	0.69
1:C:336:ILE:HD11	3:C:501:HOH:O	1.91	0.69
1:C:162:GLY:C	1:C:163:GLU:HG2	2.18	0.69
1:E:126:ASN:HD21	1:E:299:THR:H	1.39	0.68
1:F:344:ARG:NH1	1:F:344:ARG:HB2	2.09	0.68
1:D:322:GLN:HG2	1:D:323:VAL:HG23	1.74	0.68
1:B:242:GLU:HG3	3:B:454:HOH:O	1.94	0.68
1:C:156:ALA:HB2	1:C:180:LEU:HD13	1.76	0.68
1:F:180:LEU:HD13	1:F:358:LEU:HD21	1.75	0.68
1:A:311:TYR:CZ	1:B:277:ARG:HD2	2.28	0.68
1:B:188:GLY:HA2	1:B:220:TYR:CZ	2.29	0.68
1:D:168:ILE:HG12	3:D:445:HOH:O	1.94	0.68
1:E:344:ARG:HG2	1:E:344:ARG:HH11	1.59	0.68
1:E:89:LEU:HD11	1:E:125:VAL:HG11	1.75	0.68
1:E:250:LYS:HG2	1:E:279:LEU:CD1	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:HIS:HD1	1:A:343:ASP:H	1.42	0.67
1:B:347:PHE:O	1:B:351:MSE:HB2	1.95	0.67
1:D:116:ARG:HD2	1:D:294:TRP:CD1	2.30	0.67
1:C:250:LYS:HG2	1:C:279:LEU:CD1	2.25	0.67
1:F:30:MSE:HE2	1:F:381:ASP:N	2.09	0.67
1:F:340:PHE:HB3	1:F:344:ARG:HG3	1.77	0.67
1:F:153:PRO:HG2	1:F:336:ILE:HD12	1.77	0.66
1:D:141:LEU:HD23	1:D:371:LEU:HD22	1.77	0.66
1:A:188:GLY:HA2	1:A:220:TYR:CZ	2.30	0.66
1:B:30:MSE:SE	3:B:455:HOH:O	2.63	0.66
1:B:97:ILE:HG12	1:B:129:ILE:HD11	1.77	0.66
1:C:48:ARG:HG3	1:C:48:ARG:HH11	1.60	0.66
1:D:131:ASP:HB2	1:D:371:LEU:HD23	1.77	0.66
1:E:50:THR:N	1:E:74:MSE:HE1	2.10	0.66
1:E:163:GLU:OE1	1:E:167:SER:HA	1.96	0.66
1:A:95:MSE:HE3	1:B:139:MSE:SE	2.46	0.66
1:D:141:LEU:HD22	1:D:370:GLY:C	2.21	0.66
1:F:270:GLU:OE1	1:F:279:LEU:HD21	1.96	0.66
1:F:50:THR:O	1:F:74:MSE:HE1	1.96	0.66
1:F:114:ASP:HB3	1:F:117:LEU:HD22	1.77	0.65
1:D:141:LEU:CD2	1:D:371:LEU:HD22	2.27	0.65
1:E:154:MSE:HE1	1:E:363:LEU:HD13	1.78	0.64
1:B:141:LEU:HD23	1:B:371:LEU:HD13	1.78	0.64
1:B:155:ILE:HG23	1:B:336:ILE:HG21	1.79	0.64
1:F:67:THR:OG1	1:F:293:SER:HB2	1.98	0.64
1:E:30:MSE:HE2	1:E:347:PHE:CE1	2.32	0.64
1:B:30:MSE:HE1	1:B:351:MSE:SE	2.48	0.64
1:E:174:ASN:HD21	1:E:341:HIS:HE2	1.46	0.64
1:B:247:HIS:HE1	1:C:312:ASP:OD1	1.80	0.63
1:F:131:ASP:HB2	1:F:371:LEU:HD23	1.79	0.63
1:B:312:ASP:OD1	1:E:247:HIS:HE1	1.82	0.63
1:C:188:GLY:HA2	1:C:220:TYR:CZ	2.34	0.63
1:B:340:PHE:HB2	1:B:345:ASP:HB3	1.80	0.63
1:C:253:MSE:HE3	1:C:285:ILE:HG23	1.81	0.63
1:E:336:ILE:HD12	1:E:336:ILE:O	1.98	0.63
1:B:238:ARG:O	1:B:263:PRO:HG2	1.98	0.63
1:D:195:ASP:O	1:D:199:ILE:HG12	1.99	0.63
1:A:253:MSE:HE3	1:A:264:VAL:HG11	1.76	0.63
1:E:99:ARG:HG3	1:F:148:TYR:O	1.98	0.63
1:F:171:GLU:HG2	1:F:172:MSE:HE2	1.81	0.63
1:B:270:GLU:OE1	1:B:279:LEU:HD21	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:ARG:HD2	1:F:346:PRO:HD2	1.81	0.63
1:F:238:ARG:O	1:F:263:PRO:HG2	1.99	0.63
1:E:86:ALA:O	1:E:90:ILE:HG12	1.98	0.62
1:D:383:TYR:HB3	3:D:401:HOH:O	2.00	0.62
1:F:30:MSE:HE2	1:F:381:ASP:H	1.64	0.62
1:F:346:PRO:HB2	1:F:379:TYR:OH	1.99	0.62
1:B:153:PRO:HG2	1:B:336:ILE:HG12	1.81	0.62
1:B:344:ARG:HG2	1:B:344:ARG:NH1	2.14	0.62
1:C:200:THR:O	1:C:204:GLU:HG2	1.99	0.62
1:D:151:GLU:OE1	1:D:362:THR:HG21	1.99	0.62
1:E:235:LEU:HB2	1:E:237:ILE:CD1	2.28	0.62
1:C:86:ALA:HB3	1:C:87:PRO:HD3	1.82	0.62
1:E:151:GLU:CG	1:E:362:THR:HG21	2.30	0.62
1:C:376:ASN:HD21	1:C:378:ASP:HB2	1.65	0.61
1:A:20:LEU:HD11	1:A:94:ALA:HB3	1.82	0.61
1:F:126:ASN:HD21	1:F:299:THR:H	1.47	0.61
1:E:277:ARG:HH11	1:E:277:ARG:CG	2.14	0.61
1:F:155:ILE:HD11	1:F:338:GLU:HB3	1.83	0.61
1:F:348:TRP:O	1:F:355:ARG:HD3	2.00	0.61
1:A:30:MSE:H	1:A:74:MSE:HE1	1.65	0.61
1:C:48:ARG:HG2	1:C:347:PHE:CE2	2.35	0.61
1:A:277:ARG:HH12	1:E:248:ASN:HD22	1.50	0.60
1:E:268:GLN:HE21	1:E:289:ASN:HD21	1.46	0.60
1:F:253:MSE:HE2	1:F:285:ILE:CG2	2.31	0.60
1:D:126:ASN:HD21	1:D:299:THR:H	1.49	0.60
1:E:103:SER:O	1:E:106:LYS:HG2	2.01	0.60
1:B:214:ILE:HD12	1:B:237:ILE:HG21	1.82	0.60
1:D:153:PRO:HG2	1:D:336:ILE:HD12	1.82	0.60
1:E:30:MSE:HB3	1:E:384:ARG:HA	1.84	0.60
1:E:27:THR:HG21	1:E:78:ASP:OD1	2.01	0.60
1:B:235:LEU:HB2	1:B:237:ILE:CD1	2.31	0.60
1:A:126:ASN:HD21	1:A:299:THR:H	1.49	0.59
1:D:187:VAL:HG11	1:D:199:ILE:HD11	1.84	0.59
1:E:27:THR:CG2	1:E:82:HIS:NE2	2.65	0.59
1:F:154:MSE:HE1	1:F:321:PRO:HB3	1.83	0.59
1:A:253:MSE:HE1	1:A:285:ILE:HG22	1.85	0.59
1:E:200:THR:O	1:E:204:GLU:HG2	2.02	0.59
1:B:253:MSE:CE	1:B:285:ILE:CG2	2.79	0.59
1:E:168:ILE:H	1:E:168:ILE:CD1	1.99	0.59
1:C:247:HIS:HE1	1:E:312:ASP:OD1	1.86	0.59
1:E:344:ARG:HG2	1:E:344:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:PRO:O	1:B:383:TYR:HB3	2.02	0.59
1:B:277:ARG:HH11	1:B:277:ARG:CG	2.13	0.59
1:E:141:LEU:CD2	1:E:370:GLY:HA2	2.33	0.59
1:E:277:ARG:HD3	1:F:310:SER:OG	2.02	0.59
1:B:20:LEU:HB2	1:B:95:MSE:CE	2.33	0.59
1:B:119:LEU:HB3	1:B:295:SER:HA	1.85	0.58
1:E:157:ILE:HD11	1:E:338:GLU:HB2	1.84	0.58
1:C:139:MSE:HE1	1:D:95:MSE:HG3	1.85	0.58
1:D:312:ASP:OD1	1:F:247:HIS:HE1	1.87	0.58
1:F:30:MSE:H	1:F:74:MSE:CE	2.11	0.58
1:A:200:THR:O	1:A:204:GLU:HG2	2.04	0.58
1:D:48:ARG:HG3	1:D:347:PHE:CE2	2.38	0.58
1:F:48:ARG:HG2	1:F:347:PHE:HE2	1.65	0.58
1:B:56:HIS:ND1	1:B:62:ILE:HD12	2.19	0.58
1:F:149:ARG:HD2	1:F:151:GLU:O	2.04	0.58
1:B:380:ILE:HA	3:B:455:HOH:O	2.03	0.58
1:F:351:MSE:HE2	1:F:375:LEU:HG	1.85	0.58
1:C:357:LYS:HD2	3:C:466:HOH:O	2.03	0.58
1:C:49:ALA:HB1	1:C:74:MSE:HE1	1.86	0.58
1:E:114:ASP:HB3	1:E:117:LEU:HD22	1.85	0.58
1:E:155:ILE:HD13	1:E:155:ILE:H	1.69	0.58
1:A:20:LEU:HD13	1:A:57:THR:CG2	2.33	0.57
1:F:160:TYR:HB2	1:F:164:PRO:HG3	1.85	0.57
1:B:214:ILE:HD13	1:B:239:TRP:O	2.03	0.57
1:A:126:ASN:HD22	1:A:298:PRO:HD2	1.68	0.57
1:A:50:THR:O	1:A:74:MSE:CE	2.53	0.57
1:A:95:MSE:HE3	1:B:139:MSE:CE	2.35	0.57
1:D:70:GLU:HG3	1:D:77:ILE:CD1	2.35	0.57
1:F:26:GLU:OE1	1:F:54:ARG:HD3	2.04	0.57
1:D:213:CYS:SG	1:D:238:ARG:HB3	2.45	0.57
1:B:30:MSE:HE2	1:B:52:VAL:HG23	1.87	0.57
1:E:182:GLY:HA2	1:E:210:PHE:CE1	2.38	0.57
1:F:253:MSE:CE	1:F:285:ILE:CG2	2.81	0.57
1:B:67:THR:HG22	3:B:599:HOH:O	2.03	0.57
1:D:190:LEU:HB3	1:D:194:GLU:HB3	1.86	0.57
1:B:363:LEU:C	1:B:363:LEU:HD23	2.30	0.56
1:B:29:PRO:O	1:B:383:TYR:CB	2.52	0.56
1:B:340:PHE:HB2	1:B:345:ASP:CB	2.35	0.56
1:C:232:ILE:HD12	1:C:237:ILE:HG13	1.87	0.56
1:D:50:THR:N	1:D:74:MSE:HE1	2.20	0.56
1:E:277:ARG:HD2	1:F:311:TYR:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ASN:HD22	1:B:298:PRO:HD2	1.69	0.56
1:F:108:THR:CG2	1:F:119:LEU:HD12	2.33	0.56
1:B:240:PHE:HB2	1:B:262:VAL:CG2	2.35	0.56
1:D:49:ALA:O	1:D:69:ASP:HA	2.04	0.56
1:C:376:ASN:C	1:C:376:ASN:HD22	2.14	0.56
1:D:344:ARG:HH11	1:D:344:ARG:HG2	1.69	0.56
1:C:356:PRO:HG2	1:C:363:LEU:HG	1.88	0.56
1:F:154:MSE:HE2	1:F:338:GLU:C	2.31	0.56
1:C:49:ALA:HB1	1:C:74:MSE:CE	2.37	0.55
1:C:155:ILE:HD12	1:C:155:ILE:C	2.31	0.55
1:F:131:ASP:HB2	1:F:371:LEU:CD2	2.35	0.55
1:F:376:ASN:HD21	1:F:378:ASP:HB2	1.71	0.55
1:D:60:GLY:O	1:D:62:ILE:HD12	2.07	0.55
1:D:253:MSE:HE1	1:D:285:ILE:HG23	1.88	0.55
1:E:203:ARG:HG3	1:E:235:LEU:HB3	1.88	0.55
1:C:253:MSE:CE	1:C:279:LEU:HG	2.37	0.55
1:E:126:ASN:ND2	1:E:299:THR:H	2.04	0.55
1:E:138:LYS:HD3	1:E:138:LYS:N	2.21	0.55
1:E:237:ILE:HD12	1:E:237:ILE:N	2.22	0.55
1:B:20:LEU:HB2	1:B:95:MSE:HE2	1.88	0.55
1:E:347:PHE:O	1:E:351:MSE:HB2	2.06	0.55
1:B:50:THR:N	1:B:74:MSE:HE1	2.22	0.55
1:C:70:GLU:HG3	1:C:77:ILE:CD1	2.37	0.55
1:A:138:LYS:HE2	3:A:492:HOH:O	2.07	0.55
1:E:182:GLY:HA2	1:E:210:PHE:CZ	2.42	0.55
1:A:29:PRO:HA	1:A:74:MSE:HE2	1.88	0.55
1:A:348:TRP:CE2	1:A:355:ARG:HD3	2.41	0.55
1:B:253:MSE:CE	1:B:264:VAL:HG12	2.33	0.55
1:B:280:MSE:HG2	1:B:313:VAL:HG21	1.89	0.55
1:D:232:ILE:HD12	1:D:237:ILE:HG13	1.88	0.55
1:E:56:HIS:ND1	1:E:62:ILE:HD12	2.22	0.55
1:D:253:MSE:HE3	1:D:284:ALA:HB1	1.89	0.54
1:A:51:ILE:HG12	1:A:74:MSE:HE2	1.89	0.54
1:A:312:ASP:OD1	1:D:247:HIS:HE1	1.91	0.54
1:B:116:ARG:HD2	1:B:294:TRP:CD1	2.41	0.54
1:E:141:LEU:HD22	1:E:370:GLY:HA2	1.89	0.54
1:E:154:MSE:CE	1:E:363:LEU:HD13	2.37	0.54
1:B:351:MSE:HE3	1:B:375:LEU:HD22	1.89	0.54
1:E:51:ILE:HD11	1:E:74:MSE:HG3	1.89	0.54
1:B:303:ARG:HD2	3:B:448:HOH:O	2.07	0.54
1:E:238:ARG:O	1:E:263:PRO:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:LEU:HD23	1:E:370:GLY:C	2.32	0.54
1:A:310:SER:OG	1:B:277:ARG:HD3	2.08	0.54
1:A:360:ASN:N	3:A:461:HOH:O	2.39	0.54
1:B:253:MSE:HE1	1:B:285:ILE:CG2	2.32	0.54
1:C:104:GLY:O	1:C:107:VAL:HG22	2.08	0.54
1:D:268:GLN:HE21	1:D:289:ASN:HD21	1.55	0.54
1:F:188:GLY:HA2	1:F:220:TYR:CZ	2.43	0.54
1:A:30:MSE:HB3	1:A:384:ARG:HA	1.90	0.54
1:D:157:ILE:HD12	1:D:339:CYS:O	2.08	0.54
1:D:172:MSE:HG3	1:D:206:ALA:HB2	1.89	0.54
1:F:115:ARG:O	1:F:119:LEU:HD13	2.08	0.54
1:E:151:GLU:HG2	1:E:362:THR:CG2	2.36	0.53
1:E:172:MSE:HE2	1:E:172:MSE:HA	1.90	0.53
1:B:376:ASN:O	1:B:380:ILE:HG12	2.08	0.53
1:E:49:ALA:O	1:E:69:ASP:HA	2.08	0.53
1:F:301:TRP:HE3	1:F:302:LEU:HD13	1.74	0.53
1:B:67:THR:HG21	1:B:124:ALA:HA	1.89	0.53
1:C:97:ILE:HD13	1:C:130:TRP:CE2	2.42	0.53
1:E:48:ARG:HG3	1:E:347:PHE:CE2	2.44	0.53
1:C:341:HIS:HD1	1:C:343:ASP:H	1.57	0.53
1:A:20:LEU:CD1	1:A:94:ALA:HB3	2.38	0.53
1:D:344:ARG:HG2	1:D:344:ARG:O	2.07	0.53
1:E:149:ARG:HD2	1:E:151:GLU:O	2.08	0.53
1:C:31:VAL:HG22	1:C:385:VAL:HG11	1.89	0.53
1:C:153:PRO:HG2	1:C:336:ILE:HG12	1.90	0.53
1:C:238:ARG:O	1:C:263:PRO:HG2	2.08	0.53
1:A:20:LEU:HD13	1:A:57:THR:HG21	1.90	0.53
1:D:126:ASN:HD22	1:D:298:PRO:HD2	1.74	0.53
1:A:143:LYS:HD3	1:B:95:MSE:HB3	1.91	0.53
1:A:111:ILE:CD1	1:E:217:ASN:HB3	2.39	0.52
1:E:153:PRO:CG	1:E:336:ILE:HG22	2.32	0.52
1:A:269:THR:HG22	1:A:269:THR:O	2.08	0.52
1:B:237:ILE:HD12	1:B:237:ILE:N	2.24	0.52
1:C:148:TYR:O	1:D:99:ARG:NH1	2.42	0.52
1:D:153:PRO:HG2	1:D:336:ILE:HD13	1.91	0.52
1:D:383:TYR:C	3:D:401:HOH:O	2.52	0.52
1:F:155:ILE:C	1:F:155:ILE:HD12	2.34	0.52
1:A:162:GLY:C	1:A:163:GLU:HG2	2.31	0.52
1:E:171:GLU:HG2	1:E:175:TYR:CE2	2.44	0.52
1:F:190:LEU:HB3	1:F:194:GLU:OE2	2.08	0.52
1:C:126:ASN:HD22	1:C:298:PRO:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:MSE:HE3	1:C:284:ALA:HB1	1.92	0.52
1:D:138:LYS:HD3	1:D:138:LYS:N	2.24	0.52
1:A:344:ARG:HD3	1:A:344:ARG:C	2.33	0.52
1:C:141:LEU:HD22	1:C:370:GLY:C	2.34	0.52
1:E:188:GLY:HA2	1:E:220:TYR:CZ	2.44	0.52
1:F:126:ASN:ND2	1:F:299:THR:H	2.06	0.52
1:C:269:THR:HG22	1:C:269:THR:O	2.10	0.52
1:C:126:ASN:HD21	1:C:299:THR:H	1.58	0.52
1:C:253:MSE:HE1	1:C:266:ALA:HB3	1.91	0.52
1:D:189:GLY:O	1:D:190:LEU:HD12	2.09	0.52
1:E:155:ILE:HD11	1:E:338:GLU:HB3	1.91	0.52
1:F:155:ILE:CD1	1:F:338:GLU:HB3	2.40	0.52
1:E:157:ILE:HG23	1:E:186:LYS:HE2	1.92	0.52
1:B:232:ILE:HD12	1:B:237:ILE:HG12	1.92	0.52
1:E:155:ILE:HB	1:E:182:GLY:C	2.35	0.52
1:B:253:MSE:HE2	1:B:284:ALA:O	2.11	0.51
1:B:376:ASN:ND2	1:B:378:ASP:H	2.08	0.51
1:C:253:MSE:HE3	1:C:284:ALA:CB	2.40	0.51
1:A:20:LEU:HD12	1:A:20:LEU:C	2.35	0.51
1:B:157:ILE:HD12	1:B:184:LYS:HD2	1.92	0.51
1:D:360:ASN:ND2	3:D:561:HOH:O	2.43	0.51
1:A:104:GLY:O	1:A:107:VAL:HG22	2.11	0.51
1:C:29:PRO:HG2	1:C:385:VAL:O	2.10	0.51
1:C:183:VAL:HG22	1:C:184:LYS:N	2.26	0.51
1:C:319:GLU:HB2	3:C:462:HOH:O	2.11	0.51
1:D:380:ILE:O	1:D:384:ARG:HG2	2.10	0.51
1:A:340:PHE:HB3	1:A:344:ARG:HB3	1.93	0.51
1:D:70:GLU:HG3	1:D:77:ILE:HD11	1.93	0.51
1:D:363:LEU:C	1:D:363:LEU:HD23	2.34	0.51
1:A:253:MSE:CE	1:A:285:ILE:CG2	2.84	0.51
1:B:20:LEU:CB	1:B:95:MSE:HE2	2.40	0.51
1:B:149:ARG:HD2	1:B:151:GLU:O	2.11	0.51
1:D:89:LEU:CD1	1:D:125:VAL:HG11	2.40	0.51
1:B:126:ASN:HD21	1:B:299:THR:H	1.59	0.51
1:D:209:ASP:CG	1:D:209:ASP:O	2.54	0.51
1:C:185:PHE:CD2	1:C:199:ILE:HD13	2.46	0.51
1:E:116:ARG:O	1:E:120:VAL:HG23	2.11	0.51
1:E:346:PRO:HB2	1:E:379:TYR:OH	2.10	0.51
1:F:338:GLU:HG3	3:F:449:HOH:O	2.10	0.51
1:A:363:LEU:C	1:A:363:LEU:HD23	2.36	0.50
1:B:213:CYS:SG	1:B:238:ARG:HB3	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ILE:HD12	1:D:92:GLN:O	2.10	0.50
1:D:203:ARG:HD2	1:D:235:LEU:O	2.10	0.50
1:E:49:ALA:HB1	1:E:74:MSE:HE1	1.93	0.50
1:F:51:ILE:HG12	1:F:74:MSE:HE3	1.92	0.50
1:D:344:ARG:HG2	1:D:344:ARG:NH1	2.25	0.50
1:B:242:GLU:HG3	3:B:452:HOH:O	2.10	0.50
1:D:346:PRO:O	1:D:350:ASN:HB2	2.11	0.50
1:F:116:ARG:HG2	1:F:271:PHE:HE1	1.75	0.50
1:F:195:ASP:O	1:F:199:ILE:HG12	2.12	0.50
1:B:76:ASP:O	1:B:80:ILE:HG12	2.11	0.50
1:B:253:MSE:HE2	1:B:285:ILE:CG2	2.41	0.50
1:C:253:MSE:HE1	1:C:279:LEU:HG	1.92	0.50
1:D:249:ASP:O	1:D:253:MSE:HG2	2.11	0.50
1:F:67:THR:HG21	1:F:124:ALA:HA	1.94	0.50
1:A:238:ARG:O	1:A:263:PRO:HG2	2.10	0.50
1:D:49:ALA:HB1	1:D:74:MSE:HE1	1.94	0.50
1:A:48:ARG:HG2	1:A:347:PHE:CE2	2.46	0.50
1:B:253:MSE:HG3	1:B:284:ALA:HB1	1.94	0.50
1:E:338:GLU:HG3	3:E:424:HOH:O	2.12	0.50
1:C:340:PHE:HB2	1:C:345:ASP:HB3	1.94	0.50
1:D:253:MSE:CE	1:D:284:ALA:HB1	2.41	0.50
1:F:253:MSE:HE2	1:F:284:ALA:O	2.12	0.50
1:F:141:LEU:HD22	1:F:370:GLY:HA2	1.93	0.49
1:D:253:MSE:CE	1:D:285:ILE:CG2	2.89	0.49
1:D:253:MSE:HE3	1:D:284:ALA:CB	2.42	0.49
1:A:149:ARG:HD2	1:A:151:GLU:O	2.11	0.49
1:B:377:TRP:HA	1:B:380:ILE:HG12	1.94	0.49
1:D:156:ALA:HA	1:D:339:CYS:O	2.13	0.49
1:F:70:GLU:HG3	1:F:77:ILE:CD1	2.42	0.49
1:A:49:ALA:O	1:A:69:ASP:HA	2.13	0.49
1:D:250:LYS:HG2	1:D:279:LEU:CD1	2.43	0.49
1:C:162:GLY:O	1:C:163:GLU:HG2	2.11	0.49
1:F:126:ASN:ND2	1:F:298:PRO:HD2	2.25	0.49
1:F:344:ARG:HB2	1:F:344:ARG:HH11	1.78	0.49
1:A:48:ARG:HG3	1:A:48:ARG:HH11	1.77	0.49
1:D:253:MSE:HE1	1:D:285:ILE:CG2	2.43	0.49
1:D:253:MSE:HE2	1:D:279:LEU:CD1	2.42	0.49
1:E:99:ARG:HG3	1:E:99:ARG:HH11	1.77	0.49
1:E:172:MSE:HA	1:E:172:MSE:CE	2.43	0.49
1:C:28:ILE:HB	1:C:52:VAL:HB	1.95	0.49
1:F:50:THR:O	1:F:74:MSE:CE	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:ILE:HD11	1:F:74:MSE:HG3	1.94	0.48
1:B:277:ARG:CG	1:B:277:ARG:NH1	2.74	0.48
1:D:86:ALA:HB3	1:D:87:PRO:HD3	1.95	0.48
1:D:187:VAL:CG1	1:D:199:ILE:HD11	2.43	0.48
1:A:34:LEU:HD13	1:A:47:HIS:HA	1.95	0.48
1:A:239:TRP:HA	1:A:263:PRO:HG2	1.95	0.48
1:B:277:ARG:HG2	1:B:277:ARG:NH1	2.21	0.48
1:D:48:ARG:HG3	1:D:347:PHE:HE2	1.79	0.48
1:E:86:ALA:HB3	1:E:87:PRO:HD3	1.96	0.48
1:A:70:GLU:HG3	1:A:77:ILE:CD1	2.44	0.48
1:D:156:ALA:HB2	1:D:180:LEU:HD13	1.96	0.48
1:D:253:MSE:HG3	1:D:284:ALA:HB1	1.95	0.48
1:A:33:PRO:HA	1:A:47:HIS:ND1	2.27	0.48
1:E:89:LEU:CD1	1:E:125:VAL:HG11	2.43	0.48
1:E:363:LEU:HD23	1:E:363:LEU:C	2.39	0.48
1:B:77:ILE:HD13	1:B:120:VAL:HG11	1.95	0.48
1:B:357:LYS:CD	1:B:357:LYS:H	2.26	0.48
1:D:103:SER:O	1:D:106:LYS:HG2	2.12	0.48
1:A:67:THR:OG1	1:A:293:SER:HB2	2.13	0.48
1:A:247:HIS:CE1	1:F:312:ASP:OD1	2.61	0.48
1:D:104:GLY:O	1:D:107:VAL:HG22	2.13	0.48
1:E:183:VAL:HG22	1:E:184:LYS:N	2.29	0.48
1:B:129:ILE:C	1:B:129:ILE:HD12	2.39	0.48
1:C:49:ALA:O	1:C:69:ASP:HA	2.13	0.48
1:C:195:ASP:O	1:C:199:ILE:HG12	2.13	0.48
1:D:136:ALA:O	1:D:138:LYS:HE2	2.14	0.48
1:D:183:VAL:HG22	1:D:184:LYS:N	2.28	0.48
1:E:172:MSE:SE	1:E:183:VAL:HG11	2.64	0.48
1:E:141:LEU:HD12	1:E:145:TRP:CE2	2.48	0.47
1:B:188:GLY:HA2	1:B:220:TYR:CE2	2.50	0.47
1:B:214:ILE:HD13	1:B:214:ILE:H	1.77	0.47
1:B:380:ILE:O	1:B:383:TYR:CD2	2.68	0.47
1:F:266:ALA:O	1:F:288:CYS:HA	2.14	0.47
1:F:142:TRP:N	1:F:326:HIS:HD2	2.08	0.47
1:A:277:ARG:HH12	1:E:248:ASN:ND2	2.11	0.47
1:B:104:GLY:O	1:B:107:VAL:HG22	2.14	0.47
1:E:76:ASP:O	1:E:80:ILE:HD13	2.15	0.47
1:D:67:THR:HG21	1:D:124:ALA:HA	1.95	0.47
1:E:269:THR:HG22	1:E:269:THR:O	2.15	0.47
1:F:269:THR:HG22	1:F:269:THR:O	2.14	0.47
1:B:89:LEU:HD11	1:B:125:VAL:CG1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ILE:CD1	1:B:240:PHE:HA	2.45	0.47
1:F:187:VAL:HG11	1:F:199:ILE:HD11	1.97	0.47
1:E:54:ARG:HA	1:E:63:GLY:O	2.15	0.47
1:E:70:GLU:O	1:E:74:MSE:HE3	2.15	0.47
1:E:156:ALA:HB2	1:E:180:LEU:HD13	1.97	0.47
1:F:95:MSE:HE3	1:F:137:LEU:HD13	1.95	0.47
1:A:48:ARG:CZ	1:A:347:PHE:HD2	2.28	0.47
1:A:111:ILE:HD11	1:E:217:ASN:HB3	1.97	0.47
1:A:346:PRO:O	1:A:350:ASN:HB2	2.14	0.47
1:A:356:PRO:HG3	1:A:363:LEU:HD21	1.95	0.47
1:D:203:ARG:HG3	1:D:235:LEU:HB3	1.96	0.47
1:E:95:MSE:CE	1:E:95:MSE:HA	2.45	0.47
1:B:381:ASP:HA	1:B:383:TYR:HE2	1.79	0.47
1:C:187:VAL:HG11	1:C:199:ILE:HD11	1.96	0.47
1:D:253:MSE:HE1	1:D:279:LEU:HG	1.96	0.47
1:E:380:ILE:O	1:E:384:ARG:HB3	2.15	0.47
1:B:357:LYS:H	1:B:357:LYS:HD2	1.80	0.46
1:D:152:LEU:HD12	1:D:152:LEU:O	2.15	0.46
1:E:340:PHE:CD1	1:E:344:ARG:HD3	2.51	0.46
1:F:153:PRO:HG2	1:F:336:ILE:CD1	2.44	0.46
1:B:154:MSE:HE3	3:B:439:HOH:O	2.14	0.46
1:C:268:GLN:HE21	1:C:289:ASN:HD21	1.64	0.46
1:A:67:THR:HG21	1:A:124:ALA:HA	1.97	0.46
1:D:188:GLY:HA2	1:D:220:TYR:CZ	2.51	0.46
1:E:129:ILE:O	1:E:133:VAL:HG23	2.15	0.46
1:A:318:HIS:CD2	1:A:319:GLU:HG2	2.51	0.46
1:C:346:PRO:O	1:C:350:ASN:HB2	2.15	0.46
1:D:311:TYR:O	1:D:312:ASP:HB2	2.15	0.46
1:D:280:MSE:HG2	1:D:313:VAL:HG21	1.98	0.46
1:C:363:LEU:C	1:C:363:LEU:HD23	2.41	0.46
1:E:336:ILE:HD12	1:E:336:ILE:C	2.41	0.46
1:E:351:MSE:CE	1:E:375:LEU:HD22	2.38	0.46
1:B:249:ASP:O	1:B:253:MSE:HG2	2.16	0.46
1:C:99:ARG:HD3	1:D:148:TYR:O	2.16	0.46
1:E:31:VAL:O	1:E:383:TYR:HB3	2.16	0.46
1:F:183:VAL:HG12	1:F:212:ILE:HD13	1.98	0.46
1:B:357:LYS:HD2	1:B:357:LYS:N	2.31	0.45
1:E:106:LYS:HE2	1:E:106:LYS:HB3	1.72	0.45
1:E:277:ARG:CG	1:E:277:ARG:NH1	2.78	0.45
1:F:77:ILE:HD13	1:F:120:VAL:HG11	1.98	0.45
1:F:100:LEU:HD23	1:F:129:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:THR:HG22	1:F:347:PHE:CZ	2.52	0.45
1:F:351:MSE:CE	1:F:375:LEU:HG	2.45	0.45
1:E:27:THR:HG22	1:E:82:HIS:NE2	2.32	0.45
1:F:48:ARG:HD3	1:F:347:PHE:CD2	2.51	0.45
1:A:50:THR:C	1:A:74:MSE:CE	2.90	0.45
1:B:269:THR:O	1:B:269:THR:HG22	2.16	0.45
1:C:116:ARG:O	1:C:120:VAL:HG23	2.17	0.45
1:C:307:ILE:CD1	1:C:307:ILE:N	2.79	0.45
1:C:211:ILE:HD13	1:C:336:ILE:CD1	2.47	0.45
1:D:20:LEU:HB2	1:D:95:MSE:CE	2.46	0.45
1:E:203:ARG:HG2	1:E:212:ILE:HD12	1.98	0.45
1:E:342:PRO:HG3	1:E:349:TRP:CE2	2.52	0.45
1:F:86:ALA:N	1:F:87:PRO:HD2	2.32	0.45
1:F:235:LEU:HB3	1:F:237:ILE:HD11	1.99	0.45
1:F:318:HIS:HD2	3:F:415:HOH:O	1.99	0.45
1:A:126:ASN:ND2	1:A:299:THR:H	2.14	0.45
1:C:126:ASN:ND2	1:C:299:THR:H	2.15	0.45
1:D:242:GLU:HG3	3:D:465:HOH:O	2.17	0.45
1:E:126:ASN:HD22	1:E:298:PRO:HD2	1.81	0.45
1:F:142:TRP:H	1:F:326:HIS:CD2	2.23	0.45
1:C:174:ASN:HB3	3:C:455:HOH:O	2.16	0.45
1:E:266:ALA:O	1:E:288:CYS:HA	2.17	0.45
1:F:275:GLY:O	1:F:279:LEU:HD23	2.16	0.45
1:C:182:GLY:HA2	1:C:210:PHE:CE1	2.52	0.45
1:E:155:ILE:H	1:E:155:ILE:CD1	2.30	0.45
1:A:318:HIS:NE2	1:A:319:GLU:OE2	2.50	0.45
1:D:269:THR:O	1:D:269:THR:HG22	2.17	0.45
1:D:318:HIS:HD2	3:D:455:HOH:O	1.98	0.45
1:E:27:THR:HG21	1:E:82:HIS:NE2	2.31	0.45
1:A:183:VAL:HG22	1:A:184:LYS:N	2.30	0.44
1:A:363:LEU:HD23	1:A:364:THR:N	2.32	0.44
1:E:242:GLU:HG3	3:E:402:HOH:O	2.16	0.44
1:F:335:THR:C	1:F:336:ILE:HD13	2.41	0.44
1:B:48:ARG:HG3	1:B:347:PHE:CE2	2.51	0.44
1:C:186:LYS:HD2	1:C:217:ASN:HD21	1.82	0.44
1:D:340:PHE:HB2	1:D:345:ASP:HB3	1.99	0.44
1:F:179:GLY:O	1:F:361:GLY:HA2	2.17	0.44
1:F:253:MSE:HG3	1:F:284:ALA:HB1	1.98	0.44
1:D:272:SER:HB2	3:D:411:HOH:O	2.17	0.44
1:E:151:GLU:CG	1:E:362:THR:CG2	2.95	0.44
1:B:179:GLY:O	1:B:361:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ALA:O	1:B:288:CYS:HA	2.18	0.44
1:C:70:GLU:HG3	1:C:77:ILE:HD11	2.00	0.44
1:D:28:ILE:HB	1:D:52:VAL:HB	1.98	0.44
1:F:172:MSE:O	1:F:176:GLN:HG3	2.18	0.44
1:A:253:MSE:HG3	1:A:284:ALA:HB1	2.00	0.44
1:B:253:MSE:HE2	1:B:285:ILE:HG23	2.00	0.44
1:C:155:ILE:HD11	1:C:338:GLU:HB3	1.98	0.44
1:F:49:ALA:O	1:F:69:ASP:HA	2.17	0.44
1:A:77:ILE:HD13	1:A:120:VAL:HG11	1.99	0.44
1:C:157:ILE:HD12	1:C:184:LYS:HD2	1.99	0.44
1:D:69:ASP:CG	1:D:69:ASP:O	2.61	0.44
1:D:342:PRO:HG3	1:D:349:TRP:CE2	2.52	0.44
1:E:155:ILE:CD1	1:E:336:ILE:HD13	2.39	0.44
1:A:338:GLU:HG3	3:A:417:HOH:O	2.17	0.44
1:E:254:ARG:HD2	1:E:255:ASP:OD2	2.17	0.44
1:B:86:ALA:HB3	1:B:87:PRO:HD3	1.99	0.44
1:E:148:TYR:CG	1:E:332:PRO:HA	2.53	0.44
1:F:237:ILE:N	1:F:237:ILE:CD1	2.81	0.44
1:F:254:ARG:O	1:F:257:ARG:HB3	2.17	0.44
1:B:345:ASP:O	1:B:349:TRP:HD1	2.01	0.44
1:E:162:GLY:C	1:E:163:GLU:HG2	2.42	0.44
1:F:235:LEU:HB3	1:F:237:ILE:CD1	2.48	0.44
1:B:318:HIS:HD2	3:B:433:HOH:O	2.00	0.43
1:E:61:ILE:O	1:E:62:ILE:HD13	2.17	0.43
1:A:51:ILE:HG12	1:A:74:MSE:CE	2.47	0.43
1:B:56:HIS:CG	1:B:62:ILE:HD12	2.54	0.43
1:B:377:TRP:HA	1:B:380:ILE:CG1	2.47	0.43
1:A:253:MSE:CG	1:A:284:ALA:HB1	2.49	0.43
1:B:20:LEU:HG	1:B:57:THR:HG21	1.99	0.43
1:B:29:PRO:O	1:B:383:TYR:HB2	2.18	0.43
1:D:182:GLY:HA2	1:D:210:PHE:CZ	2.53	0.43
1:B:240:PHE:HB2	1:B:262:VAL:HG21	1.99	0.43
1:C:103:SER:O	1:C:106:LYS:HG2	2.18	0.43
1:D:116:ARG:O	1:D:120:VAL:HG23	2.18	0.43
1:E:250:LYS:HE3	3:E:529:HOH:O	2.17	0.43
1:E:97:ILE:HD12	1:E:97:ILE:H	1.82	0.43
1:F:95:MSE:HE1	1:F:136:ALA:CB	2.48	0.43
1:A:99:ARG:HD3	1:B:148:TYR:O	2.19	0.43
1:B:336:ILE:HG22	1:B:337:ALA:O	2.19	0.43
1:C:253:MSE:HG3	1:C:284:ALA:HB1	2.01	0.43
1:D:30:MSE:HE2	1:D:347:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:GLU:HB2	1:E:320:GLU:H	1.63	0.43
1:B:383:TYR:CD2	1:B:383:TYR:N	2.85	0.43
1:A:79:ARG:CZ	1:A:79:ARG:HB2	2.48	0.43
1:B:20:LEU:HD22	1:B:95:MSE:HE1	2.01	0.43
1:E:104:GLY:O	1:E:107:VAL:HG22	2.19	0.43
1:F:50:THR:C	1:F:74:MSE:CE	2.91	0.43
1:A:287:VAL:HG22	1:A:314:GLN:HB2	2.00	0.43
1:B:381:ASP:HA	1:B:383:TYR:CE2	2.54	0.43
1:D:161:TYR:CE1	1:D:190:LEU:HD13	2.54	0.43
1:F:270:GLU:CD	1:F:279:LEU:HD21	2.43	0.43
1:A:188:GLY:HA2	1:A:220:TYR:CE2	2.53	0.43
1:E:70:GLU:HG3	1:E:77:ILE:CD1	2.49	0.43
1:A:319:GLU:HB2	3:A:456:HOH:O	2.19	0.42
1:B:116:ARG:O	1:B:120:VAL:HG23	2.19	0.42
1:B:253:MSE:CE	1:B:284:ALA:O	2.67	0.42
1:B:253:MSE:HE2	1:B:284:ALA:C	2.44	0.42
1:F:141:LEU:CD2	1:F:370:GLY:C	2.92	0.42
1:B:30:MSE:HE3	1:B:50:THR:CG2	2.49	0.42
1:F:249:ASP:O	1:F:253:MSE:HG2	2.19	0.42
1:A:155:ILE:HG23	1:A:336:ILE:HG21	2.01	0.42
1:B:344:ARG:HG2	1:B:344:ARG:O	2.18	0.42
1:C:211:ILE:HD13	1:C:336:ILE:HD13	2.02	0.42
1:F:154:MSE:HE3	1:F:337:ALA:CB	2.49	0.42
1:A:168:ILE:O	1:A:172:MSE:HG2	2.19	0.42
1:B:156:ALA:HB2	1:B:180:LEU:CD1	2.42	0.42
1:B:376:ASN:C	1:B:376:ASN:HD22	2.25	0.42
1:B:382:GLN:H	1:B:383:TYR:HD2	1.67	0.42
1:C:33:PRO:HA	1:C:47:HIS:ND1	2.34	0.42
1:C:376:ASN:C	1:C:376:ASN:ND2	2.76	0.42
1:D:189:GLY:C	1:D:190:LEU:HD12	2.44	0.42
1:D:359:ASN:C	1:D:359:ASN:HD22	2.26	0.42
1:E:346:PRO:O	1:E:350:ASN:HB2	2.19	0.42
1:F:203:ARG:NH1	1:F:235:LEU:O	2.51	0.42
1:C:188:GLY:HA2	1:C:220:TYR:CE1	2.55	0.42
1:A:126:ASN:ND2	1:A:298:PRO:HD2	2.33	0.42
1:A:156:ALA:O	1:A:183:VAL:HG23	2.19	0.42
1:A:95:MSE:CE	1:B:139:MSE:SE	3.17	0.42
1:D:241:GLU:O	1:D:242:GLU:C	2.63	0.42
1:E:125:VAL:O	1:E:129:ILE:HG13	2.19	0.42
1:E:152:LEU:O	1:E:152:LEU:HD12	2.20	0.42
1:B:49:ALA:HB1	1:B:74:MSE:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLY:HA3	1:B:132:ALA:HB2	2.02	0.42
1:C:187:VAL:CG1	1:C:199:ILE:HD11	2.50	0.42
1:C:253:MSE:CG	1:C:284:ALA:HB1	2.49	0.42
1:D:20:LEU:HB2	1:D:95:MSE:HE2	2.01	0.42
1:E:333:HIS:ND1	1:E:333:HIS:N	2.68	0.42
1:F:125:VAL:O	1:F:129:ILE:HG13	2.19	0.42
1:C:31:VAL:HG22	1:C:385:VAL:CG1	2.50	0.42
1:D:131:ASP:CB	1:D:371:LEU:HD23	2.48	0.42
1:E:149:ARG:O	1:E:329:ALA:HB1	2.20	0.42
1:F:340:PHE:HB2	1:F:345:ASP:HB2	2.02	0.42
1:D:211:ILE:N	1:D:211:ILE:HD12	2.35	0.41
1:E:95:MSE:HE2	1:E:95:MSE:HA	2.02	0.41
1:F:142:TRP:CH2	1:F:143:LYS:HE3	2.55	0.41
1:F:210:PHE:HD2	1:F:212:ILE:HD11	1.85	0.41
1:B:51:ILE:O	1:B:66:TYR:HA	2.21	0.41
1:E:232:ILE:HD12	1:E:237:ILE:HG12	2.01	0.41
1:A:125:VAL:O	1:A:129:ILE:HG13	2.20	0.41
1:A:141:LEU:CD2	1:A:371:LEU:HD13	2.50	0.41
1:A:238:ARG:O	1:A:263:PRO:CG	2.68	0.41
1:C:157:ILE:HB	1:C:340:PHE:CD1	2.55	0.41
1:D:376:ASN:ND2	1:D:378:ASP:HB2	2.28	0.41
1:A:253:MSE:HE2	1:A:284:ALA:O	2.20	0.41
1:C:156:ALA:HA	1:C:339:CYS:O	2.21	0.41
1:C:253:MSE:CE	1:C:285:ILE:HG23	2.49	0.41
1:D:86:ALA:N	1:D:87:PRO:CD	2.84	0.41
1:F:178:LEU:HB3	1:F:180:LEU:HD23	2.03	0.41
1:F:347:PHE:O	1:F:351:MSE:HB2	2.20	0.41
1:F:363:LEU:C	1:F:363:LEU:HD12	2.45	0.41
1:B:318:HIS:O	1:B:319:GLU:HG2	2.21	0.41
1:C:48:ARG:HG2	1:C:347:PHE:CD2	2.55	0.41
1:F:51:ILE:HD13	1:F:74:MSE:HE2	2.01	0.41
1:B:126:ASN:ND2	1:B:298:PRO:HD2	2.33	0.41
1:B:291:ASP:HB2	1:B:318:HIS:HB3	2.03	0.41
1:D:340:PHE:CD1	1:D:344:ARG:HD3	2.56	0.41
1:E:190:LEU:HB3	1:E:194:GLU:OE2	2.20	0.41
1:C:30:MSE:HB3	1:C:384:ARG:HA	2.02	0.41
1:D:346:PRO:HB2	1:D:379:TYR:OH	2.21	0.41
1:F:50:THR:C	1:F:74:MSE:HE3	2.46	0.41
1:A:86:ALA:HB3	1:A:87:PRO:HD3	2.02	0.41
1:C:266:ALA:O	1:C:288:CYS:HA	2.21	0.41
1:E:99:ARG:HG3	1:E:99:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:318:HIS:HD2	3:E:450:HOH:O	2.04	0.41
1:F:335:THR:O	1:F:336:ILE:HD13	2.21	0.41
1:A:116:ARG:O	1:A:120:VAL:HG23	2.20	0.41
1:A:171:GLU:HG2	1:A:175:TYR:CE2	2.56	0.41
1:A:335:THR:O	1:A:336:ILE:HD13	2.21	0.41
1:A:29:PRO:CA	1:A:74:MSE:HE2	2.51	0.40
1:B:319:GLU:HG3	1:B:320:GLU:HG2	2.03	0.40
1:B:376:ASN:ND2	1:B:376:ASN:C	2.79	0.40
1:C:48:ARG:HH11	1:C:48:ARG:CG	2.28	0.40
1:C:362:THR:CG2	1:C:363:LEU:N	2.84	0.40
1:D:50:THR:HG22	1:D:347:PHE:CZ	2.56	0.40
1:D:319:GLU:HB2	1:D:320:GLU:H	1.70	0.40
1:D:371:LEU:HB3	1:D:373:TRP:CD1	2.56	0.40
1:F:141:LEU:HD22	1:F:370:GLY:C	2.46	0.40
1:A:318:HIS:CE1	1:A:319:GLU:OE2	2.75	0.40
1:D:148:TYR:CG	1:D:332:PRO:HA	2.56	0.40
1:E:27:THR:O	1:E:27:THR:HG23	2.22	0.40
1:E:253:MSE:CG	1:E:284:ALA:HB1	2.51	0.40
1:F:371:LEU:HB3	1:F:373:TRP:CD1	2.56	0.40
1:A:182:GLY:HA2	1:A:210:PHE:CZ	2.56	0.40
1:B:70:GLU:HG3	1:B:77:ILE:CD1	2.51	0.40
1:D:157:ILE:CG2	1:D:186:LYS:HE2	2.51	0.40
1:D:171:GLU:HG2	1:D:175:TYR:CE2	2.57	0.40
1:C:111:ILE:HD12	1:C:111:ILE:N	2.37	0.40
1:F:319:GLU:HB2	3:F:613:HOH:O	2.22	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	351/398 (88%)	340 (97%)	10 (3%)	1 (0%)	36 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	345/398 (87%)	328 (95%)	16 (5%)	1 (0%)	36	34
1	C	353/398 (89%)	344 (98%)	8 (2%)	1 (0%)	36	34
1	D	346/398 (87%)	331 (96%)	14 (4%)	1 (0%)	36	34
1	E	349/398 (88%)	333 (95%)	14 (4%)	2 (1%)	21	15
1	F	345/398 (87%)	325 (94%)	18 (5%)	2 (1%)	21	15
All	All	2089/2388 (88%)	2001 (96%)	80 (4%)	8 (0%)	30	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	319	GLU
1	A	319	GLU
1	F	319	GLU
1	B	187	VAL
1	C	319	GLU
1	D	110	ASP
1	E	187	VAL
1	F	164	PRO

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	287/313 (92%)	280 (98%)	7 (2%)	43	47
1	B	282/313 (90%)	267 (95%)	15 (5%)	20	17
1	C	288/313 (92%)	281 (98%)	7 (2%)	43	47
1	D	283/313 (90%)	273 (96%)	10 (4%)	32	32
1	E	285/313 (91%)	267 (94%)	18 (6%)	16	11
1	F	280/313 (90%)	267 (95%)	13 (5%)	24	22
All	All	1705/1878 (91%)	1635 (96%)	70 (4%)	27	26

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LYS
1	A	141	LEU
1	A	152	LEU
1	A	163	GLU
1	A	338	GLU
1	A	371	LEU
1	A	375	LEU
1	B	129	ILE
1	B	138	LYS
1	B	141	LEU
1	B	152	LEU
1	B	154	MSE
1	B	163	GLU
1	B	203	ARG
1	B	209	ASP
1	B	214	ILE
1	B	262	VAL
1	B	295	SER
1	B	343	ASP
1	B	357	LYS
1	B	371	LEU
1	B	383	TYR
1	C	48	ARG
1	C	141	LEU
1	C	152	LEU
1	C	172	MSE
1	C	279	LEU
1	C	307	ILE
1	C	338	GLU
1	D	119	LEU
1	D	138	LYS
1	D	141	LEU
1	D	163	GLU
1	D	172	MSE
1	D	194	GLU
1	D	228	LEU
1	D	279	LEU
1	D	295	SER
1	D	384	ARG
1	E	67	THR
1	E	95	MSE
1	E	99	ARG
1	E	138	LYS

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Mol	Chain	Res	Type
1	E	141	LEU
1	E	152	LEU
1	E	155	ILE
1	E	163	GLU
1	E	168	ILE
1	E	172	MSE
1	E	203	ARG
1	E	221	LYS
1	E	279	LEU
1	E	294	TRP
1	E	295	SER
1	E	338	GLU
1	E	371	LEU
1	E	382	GLN
1	F	95	MSE
1	F	111	ILE
1	F	117	LEU
1	F	137	LEU
1	F	141	LEU
1	F	203	ARG
1	F	235	LEU
1	F	237	ILE
1	F	262	VAL
1	F	268	GLN
1	F	302	LEU
1	F	338	GLU
1	F	358	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	174	ASN
1	A	217	ASN
1	A	247	HIS
1	A	268	GLN
1	A	359	ASN
1	A	360	ASN
1	A	376	ASN
1	A	382	GLN
1	B	126	ASN
1	B	174	ASN

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Mol	Chain	Res	Type
1	B	217	ASN
1	B	247	HIS
1	B	318	HIS
1	B	350	ASN
1	B	359	ASN
1	B	360	ASN
1	B	376	ASN
1	C	71	HIS
1	C	92	GLN
1	C	126	ASN
1	C	174	ASN
1	C	217	ASN
1	C	247	HIS
1	C	359	ASN
1	C	360	ASN
1	C	376	ASN
1	C	382	GLN
1	D	92	GLN
1	D	126	ASN
1	D	247	HIS
1	D	318	HIS
1	D	350	ASN
1	D	359	ASN
1	D	360	ASN
1	D	376	ASN
1	E	92	GLN
1	E	126	ASN
1	E	173	HIS
1	E	174	ASN
1	E	247	HIS
1	E	248	ASN
1	E	318	HIS
1	E	359	ASN
1	E	382	GLN
1	F	126	ASN
1	F	174	ASN
1	F	217	ASN
1	F	236	ASN
1	F	247	HIS
1	F	248	ASN
1	F	259	GLN
1	F	326	HIS

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Mol	Chain	Res	Type
1	F	376	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	345/398 (86%)	-0.01	11 (3%)	50	54	7, 16, 31, 41	0
1	B	339/398 (85%)	0.38	21 (6%)	26	30	8, 21, 38, 43	0
1	C	347/398 (87%)	-0.01	10 (2%)	53	57	7, 16, 31, 40	0
1	D	340/398 (85%)	0.32	21 (6%)	26	30	8, 21, 37, 44	0
1	E	343/398 (86%)	0.42	21 (6%)	27	31	10, 22, 37, 43	0
1	F	339/398 (85%)	0.41	25 (7%)	20	23	7, 22, 38, 48	0
All	All	2053/2388 (85%)	0.25	109 (5%)	32	36	7, 20, 36, 48	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	69	ASP	5.8
1	F	163	GLU	5.3
1	A	35	ALA	4.6
1	E	164	PRO	4.4
1	F	162	GLY	4.2
1	E	67	THR	3.9
1	D	357	LYS	3.9
1	E	168	ILE	3.8
1	E	32	ALA	3.7
1	D	69	ASP	3.7
1	E	111	ILE	3.6
1	C	69	ASP	3.6
1	B	294	TRP	3.5
1	F	165	LEU	3.5
1	E	162	GLY	3.5
1	B	59	ALA	3.4
1	A	165	LEU	3.4
1	D	164	PRO	3.4
1	B	165	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	68	GLY	3.3
1	B	383	TYR	3.2
1	B	381	ASP	3.2
1	F	164	PRO	3.1
1	E	69	ASP	3.1
1	D	344	ARG	3.1
1	F	19	GLY	3.0
1	A	33	PRO	3.0
1	F	382	GLN	3.0
1	A	69	ASP	3.0
1	C	386	SER	3.0
1	E	165	LEU	3.0
1	B	380	ILE	3.0
1	E	209	ASP	3.0
1	D	294	TRP	3.0
1	D	165	LEU	2.9
1	B	209	ASP	2.9
1	C	209	ASP	2.9
1	A	47	HIS	2.9
1	A	385	VAL	2.8
1	F	344	ARG	2.8
1	E	60	GLY	2.8
1	F	67	THR	2.8
1	F	112	LEU	2.8
1	D	31	VAL	2.8
1	E	344	ARG	2.7
1	C	294	TRP	2.7
1	A	67	THR	2.7
1	F	354	ASN	2.7
1	F	70	GLU	2.7
1	B	69	ASP	2.7
1	A	59	ALA	2.7
1	B	336	ILE	2.7
1	D	160	TYR	2.6
1	F	178	LEU	2.6
1	B	343	ASP	2.6
1	F	381	ASP	2.6
1	C	357	LYS	2.6
1	D	209	ASP	2.6
1	D	71	HIS	2.5
1	F	48	ARG	2.5
1	D	166	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	112	LEU	2.5
1	E	382	GLN	2.4
1	E	138	LYS	2.4
1	C	68	GLY	2.4
1	F	377	TRP	2.4
1	E	343	ASP	2.4
1	F	209	ASP	2.4
1	D	383	TYR	2.3
1	C	47	HIS	2.3
1	B	382	GLN	2.3
1	A	60	GLY	2.3
1	E	294	TRP	2.3
1	B	163	GLU	2.2
1	B	75	PHE	2.2
1	D	67	THR	2.2
1	A	34	LEU	2.2
1	E	386	SER	2.2
1	E	27	THR	2.2
1	F	138	LYS	2.2
1	D	112	LEU	2.2
1	D	75	PHE	2.2
1	B	32	ALA	2.2
1	E	59	ALA	2.2
1	B	112	LEU	2.2
1	B	48	ARG	2.2
1	E	70	GLU	2.1
1	F	111	ILE	2.1
1	E	166	GLY	2.1
1	B	341	HIS	2.1
1	B	205	ALA	2.1
1	A	112	LEU	2.1
1	C	33	PRO	2.1
1	F	347	PHE	2.1
1	D	49	ALA	2.1
1	E	360	ASN	2.1
1	D	343	ASP	2.1
1	B	164	PRO	2.1
1	F	342	PRO	2.1
1	C	35	ALA	2.1
1	F	151	GLU	2.0
1	B	67	THR	2.0
1	D	346	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	189	GLY	2.0
1	D	204	GLU	2.0
1	D	59	ALA	2.0
1	B	357	LYS	2.0
1	F	87	PRO	2.0
1	D	68	GLY	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	MG	A	397	1/1	0.93	0.06	19,19,19,19	0
2	MG	F	397	1/1	0.94	0.12	26,26,26,26	0
2	MG	E	397	1/1	0.96	0.07	29,29,29,29	0
2	MG	D	397	1/1	0.97	0.12	24,24,24,24	0
2	MG	B	397	1/1	0.97	0.12	25,25,25,25	0
2	MG	C	397	1/1	0.97	0.08	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.