



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:40 PM UTC

PDB ID : 7EBE / pdb_00007ebe
Title : Crystal structure of Isocitrate lyase-1 from *Candida albicans*
Authors : Hiragi, K.; Nishio, K.; Moriyama, S.; Hamaguchi, T.; Mizoguchi, A.; Yonekura, K.; Tani, K.; Mizushima, T.
Deposited on : 2021-03-09
Resolution : 2.69 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

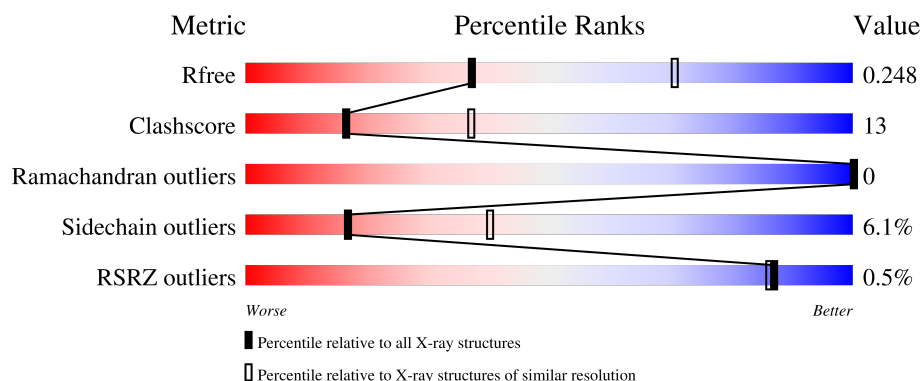
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	556	
1	B	556	
1	C	556	
1	D	556	
1	E	556	

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Mol	Chain	Length	Quality of chain
1	F	556	
1	G	556	
1	H	556	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMT	B	603	-	-	X	-
3	FMT	H	603	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34327 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 Isocitrate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			4289	2728	736	810	15			
1	B	540	Total	C	N	O	S	0	0	0
			4252	2703	730	805	14			
1	C	535	Total	C	N	O	S	0	0	0
			4219	2683	725	797	14			
1	D	541	Total	C	N	O	S	0	0	0
			4265	2712	733	806	14			
1	E	542	Total	C	N	O	S	0	0	0
			4276	2720	734	808	14			
1	F	543	Total	C	N	O	S	0	0	0
			4281	2723	735	809	14			
1	G	535	Total	C	N	O	S	0	0	0
			4212	2677	725	796	14			
1	H	533	Total	C	N	O	S	0	0	0
			4191	2665	723	789	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q59RB8
A	-4	HIS	-	expression tag	UNP Q59RB8
A	-3	HIS	-	expression tag	UNP Q59RB8
A	-2	HIS	-	expression tag	UNP Q59RB8
A	-1	HIS	-	expression tag	UNP Q59RB8
A	0	HIS	-	expression tag	UNP Q59RB8
B	-5	HIS	-	expression tag	UNP Q59RB8
B	-4	HIS	-	expression tag	UNP Q59RB8
B	-3	HIS	-	expression tag	UNP Q59RB8
B	-2	HIS	-	expression tag	UNP Q59RB8
B	-1	HIS	-	expression tag	UNP Q59RB8
B	0	HIS	-	expression tag	UNP Q59RB8
C	-5	HIS	-	expression tag	UNP Q59RB8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP Q59RB8
C	-3	HIS	-	expression tag	UNP Q59RB8
C	-2	HIS	-	expression tag	UNP Q59RB8
C	-1	HIS	-	expression tag	UNP Q59RB8
C	0	HIS	-	expression tag	UNP Q59RB8
D	-5	HIS	-	expression tag	UNP Q59RB8
D	-4	HIS	-	expression tag	UNP Q59RB8
D	-3	HIS	-	expression tag	UNP Q59RB8
D	-2	HIS	-	expression tag	UNP Q59RB8
D	-1	HIS	-	expression tag	UNP Q59RB8
D	0	HIS	-	expression tag	UNP Q59RB8
E	-5	HIS	-	expression tag	UNP Q59RB8
E	-4	HIS	-	expression tag	UNP Q59RB8
E	-3	HIS	-	expression tag	UNP Q59RB8
E	-2	HIS	-	expression tag	UNP Q59RB8
E	-1	HIS	-	expression tag	UNP Q59RB8
E	0	HIS	-	expression tag	UNP Q59RB8
F	-5	HIS	-	expression tag	UNP Q59RB8
F	-4	HIS	-	expression tag	UNP Q59RB8
F	-3	HIS	-	expression tag	UNP Q59RB8
F	-2	HIS	-	expression tag	UNP Q59RB8
F	-1	HIS	-	expression tag	UNP Q59RB8
F	0	HIS	-	expression tag	UNP Q59RB8
G	-5	HIS	-	expression tag	UNP Q59RB8
G	-4	HIS	-	expression tag	UNP Q59RB8
G	-3	HIS	-	expression tag	UNP Q59RB8
G	-2	HIS	-	expression tag	UNP Q59RB8
G	-1	HIS	-	expression tag	UNP Q59RB8
G	0	HIS	-	expression tag	UNP Q59RB8
H	-5	HIS	-	expression tag	UNP Q59RB8
H	-4	HIS	-	expression tag	UNP Q59RB8
H	-3	HIS	-	expression tag	UNP Q59RB8
H	-2	HIS	-	expression tag	UNP Q59RB8
H	-1	HIS	-	expression tag	UNP Q59RB8
H	0	HIS	-	expression tag	UNP Q59RB8

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

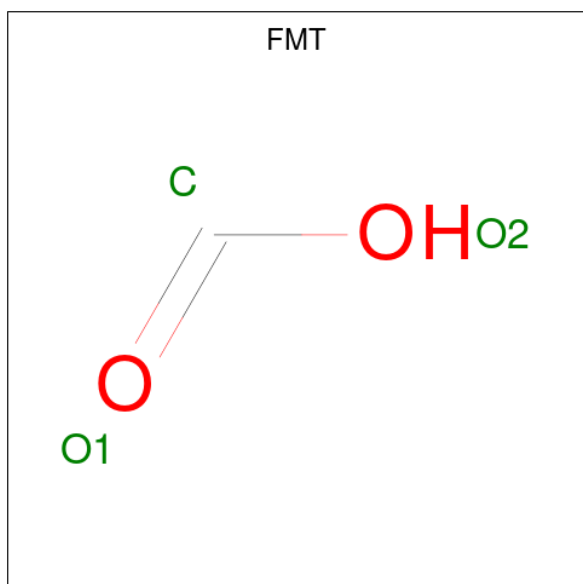
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

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

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 3	C 1	O 2	0	0
3	A	1	Total 3	C 1	O 2	0	0
3	B	1	Total 3	C 1	O 2	0	0
3	B	1	Total 3	C 1	O 2	0	0
3	C	1	Total 3	C 1	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0

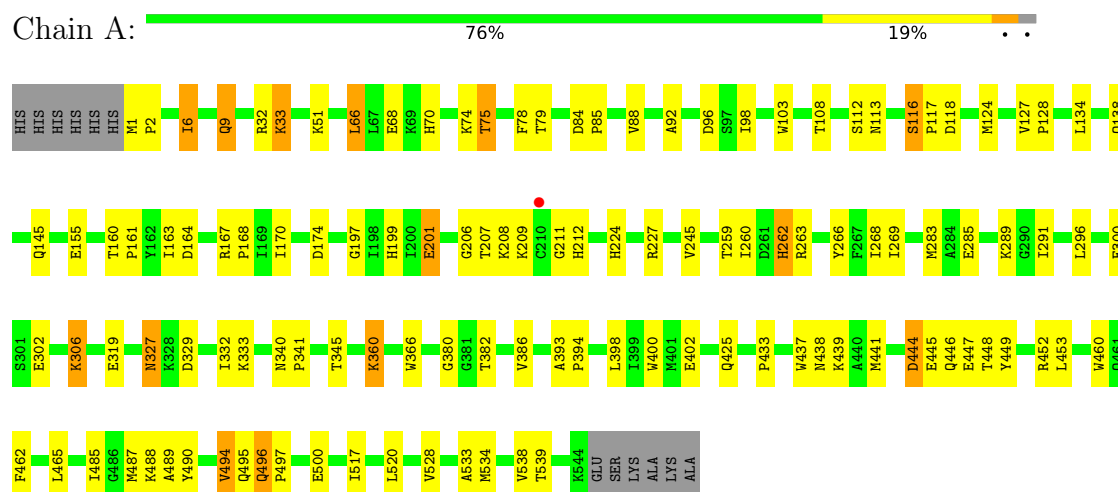
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0
4	B	38	Total O 38 38	0	0
4	C	56	Total O 56 56	0	0
4	D	29	Total O 29 29	0	0
4	E	29	Total O 29 29	0	0
4	F	22	Total O 22 22	0	0
4	G	52	Total O 52 52	0	0
4	H	40	Total O 40 40	0	0

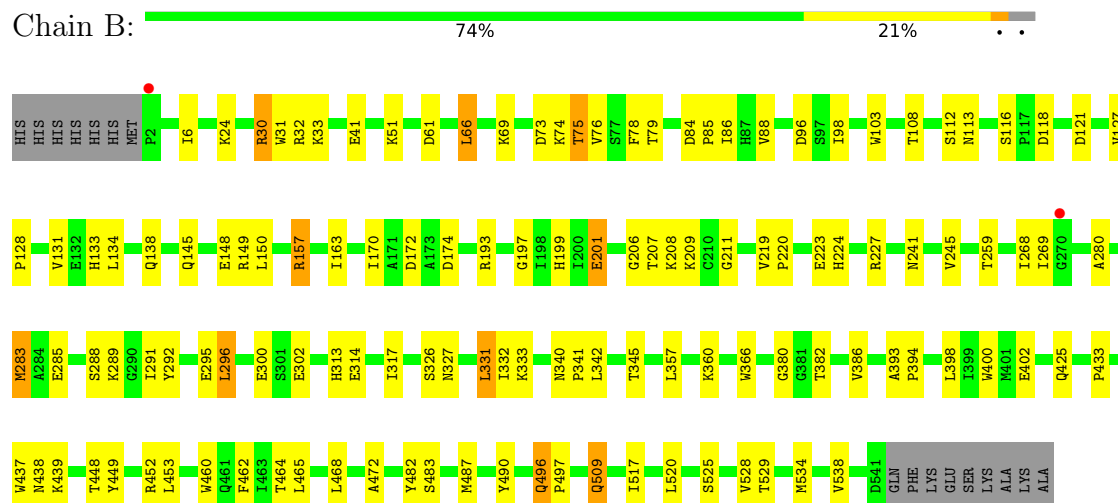
3 Residue-property plots

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.

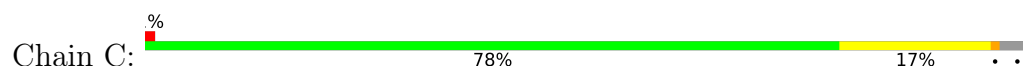
• Molecule 1: Isocitrate lyase

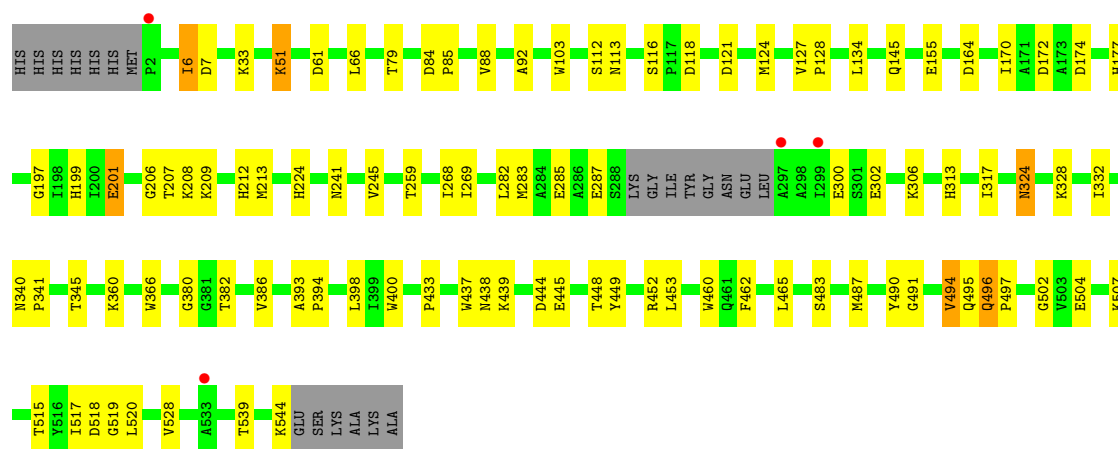


• Molecule 1: Isocitrate lyase



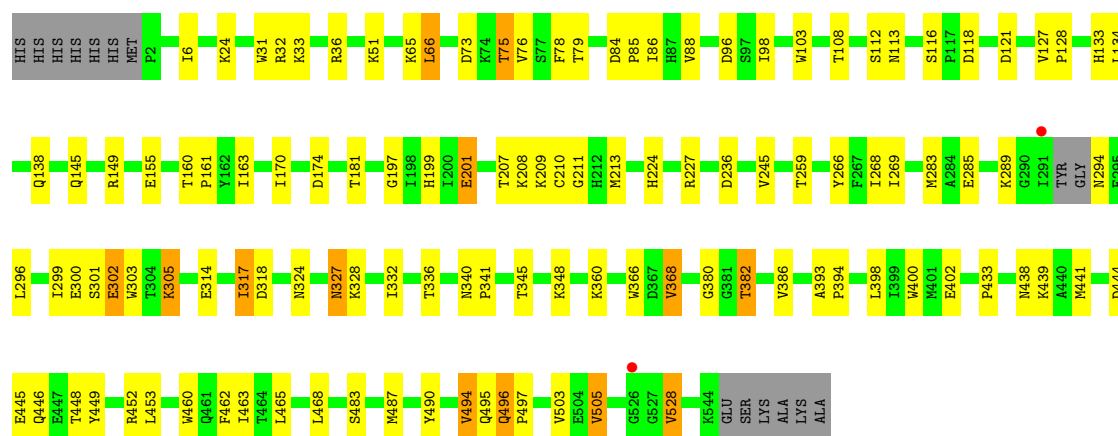
• Molecule 1: Isocitrate lyase





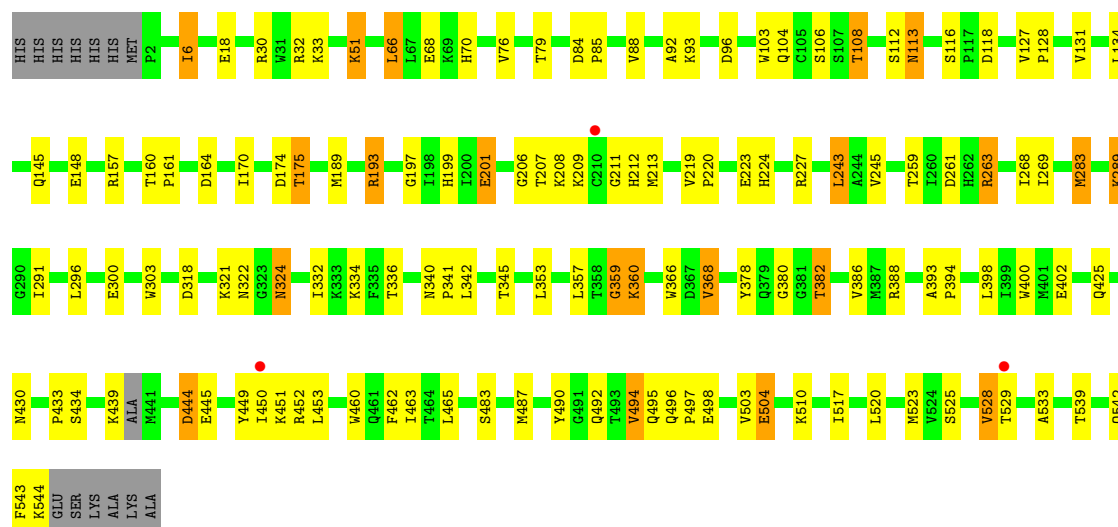
• Molecule 1: Isocitrate lyase

Chain D: 76% 19% . .

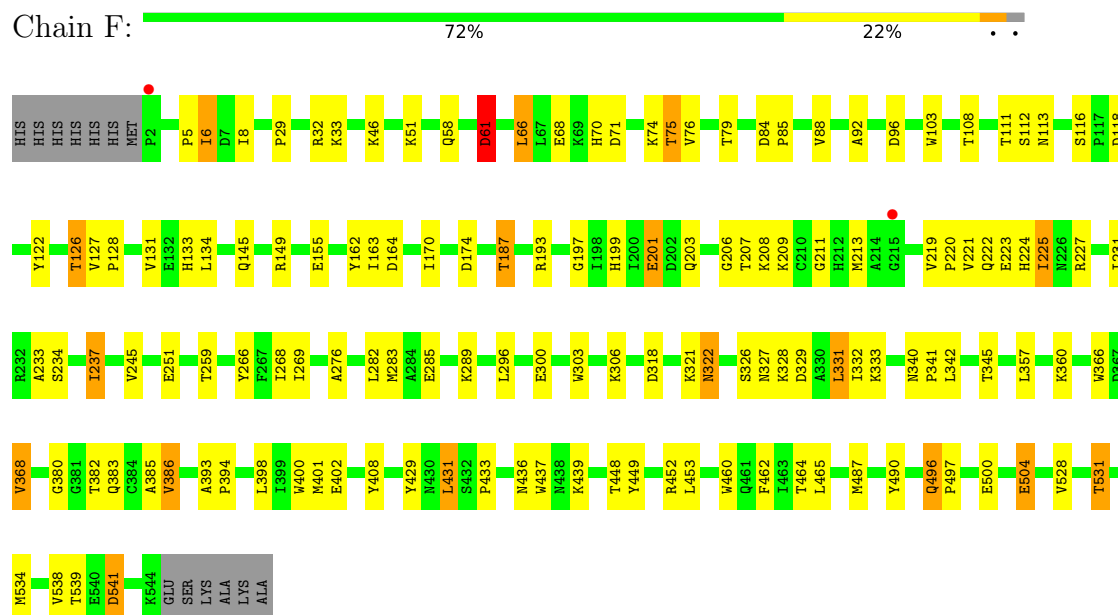


• Molecule 1: Isocitrate lyase

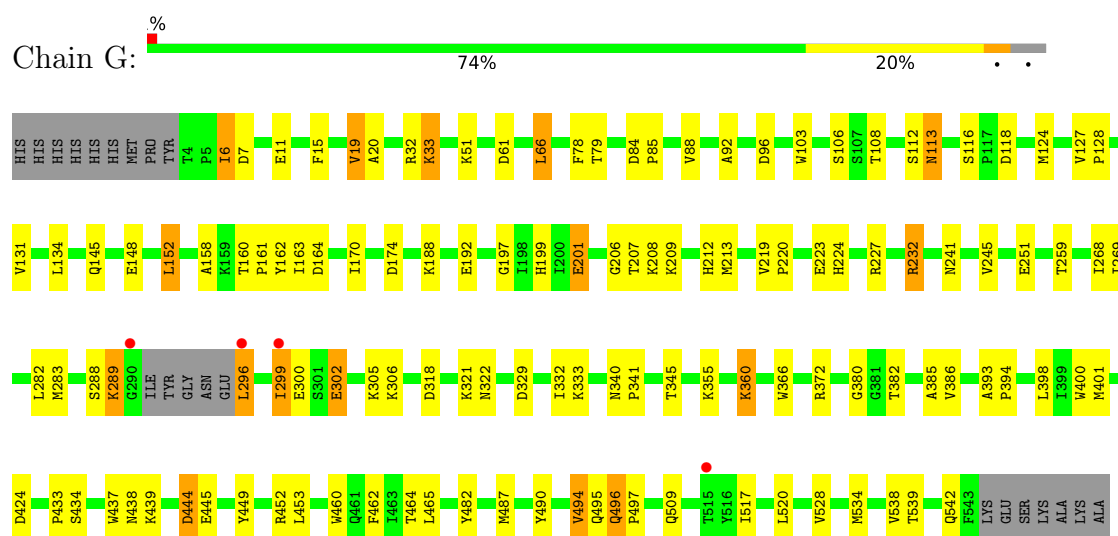
Chain E: 73% 20% . .



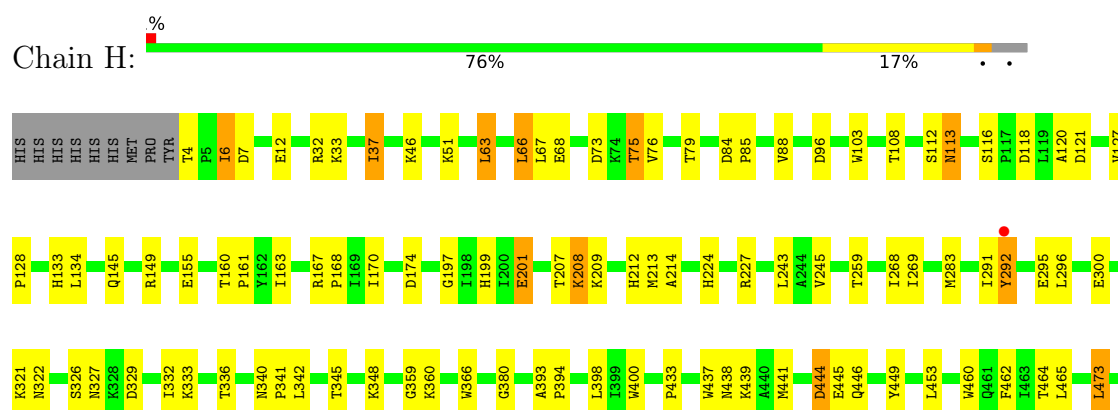
- Molecule 1: Isocitrate lyase

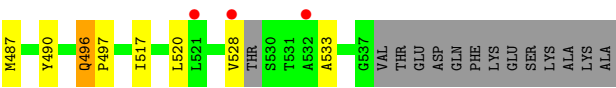


- Molecule 1: Isocitrate lyase



- Molecule 1: Isocitrate lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.97Å 139.91Å 200.30Å 90.00° 92.55° 90.00°	Depositor
Resolution (Å)	47.11 – 2.69 47.11 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.11-2.69) 99.5 (47.11-2.69)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.215 , 0.248 0.217 , 0.248	Depositor DCC
R_{free} test set	6148 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34327	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.85% 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: FMT, 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	0.29	0/4389	0.63	0/5938
1	B	0.29	0/4351	0.63	0/5888
1	C	0.29	0/4317	0.63	0/5840
1	D	0.29	0/4363	0.63	0/5901
1	E	0.28	0/4375	0.64	0/5917
1	F	0.29	0/4381	0.64	1/5927 (0.0%)
1	G	0.28	0/4308	0.63	0/5827
1	H	0.29	0/4287	0.64	0/5798
All	All	0.29	0/34771	0.64	1/47036 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	4
1	D	0	2
1	E	0	4
1	F	0	3
1	G	0	3
1	H	0	3
All	All	0	25

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	61	ASP	N-CA-CB	5.34	117.75	110.01

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	GLY	Peptide
1	A	360	LYS	Peptide
1	A	380	GLY	Peptide
1	B	206	GLY	Peptide
1	B	360	LYS	Peptide
1	B	380	GLY	Peptide
1	C	206	GLY	Peptide
1	C	360	LYS	Peptide
1	C	380	GLY	Peptide
1	C	502	GLY	Peptide
1	D	360	LYS	Peptide
1	D	380	GLY	Peptide
1	E	206	GLY	Peptide
1	E	359	GLY	Peptide
1	E	360	LYS	Peptide
1	E	380	GLY	Peptide
1	F	206	GLY	Peptide
1	F	360	LYS	Peptide
1	F	380	GLY	Peptide
1	G	206	GLY	Peptide
1	G	360	LYS	Peptide
1	G	380	GLY	Peptide
1	H	359	GLY	Peptide
1	H	360	LYS	Peptide
1	H	380	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4289	0	4239	107	1
1	B	4252	0	4198	134	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4219	0	4165	84	0
1	D	4265	0	4215	109	1
1	E	4276	0	4222	148	0
1	F	4281	0	4228	151	1
1	G	4212	0	4162	142	0
1	H	4191	0	4143	105	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	6	0	2	0	0
3	B	6	0	2	2	0
3	C	6	0	2	0	0
3	D	6	0	2	1	0
3	G	6	0	2	1	0
3	H	6	0	2	2	0
4	A	32	0	0	2	0
4	B	38	0	0	2	0
4	C	56	0	0	7	0
4	D	29	0	0	0	0
4	E	29	0	0	0	0
4	F	22	0	0	2	0
4	G	52	0	0	1	0
4	H	40	0	0	0	0
All	All	34327	0	33584	870	3

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 13.

All (870) 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:B:149:ARG:O	1:B:157:ARG:NH1	1.65	1.28
1:F:29:PRO:O	1:F:32:ARG:HD3	1.41	1.21
1:G:219:VAL:HG22	1:G:220:PRO:HD2	1.32	1.11
1:E:219:VAL:HG22	1:E:220:PRO:HD2	1.32	1.10
1:B:296:LEU:CD2	1:D:528:VAL:HG21	1.79	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:533:ALA:HB1	1:G:213:MET:HE3	1.32	1.08
1:E:463:ILE:CD1	1:G:487:MET:HE1	1.83	1.07
1:E:463:ILE:HD11	1:G:487:MET:HE1	1.07	1.06
1:A:533:ALA:HB1	1:C:213:MET:HE3	1.37	1.06
1:B:487:MET:HE1	1:D:463:ILE:CD1	1.84	1.06
1:F:276:ALA:HA	1:F:306:LYS:NZ	1.71	1.05
1:B:296:LEU:HD22	1:D:528:VAL:HG21	1.33	1.05
1:B:464:THR:HG21	3:B:603:FMT:O2	1.55	1.05
1:F:276:ALA:HA	1:F:306:LYS:HZ1	1.14	1.05
1:G:232:ARG:HG2	1:G:232:ARG:HH21	1.14	1.04
1:F:219:VAL:HG12	1:F:220:PRO:HD2	1.38	1.04
1:A:441:MET:HE3	1:A:445:GLU:HB3	1.36	1.03
1:E:283:MET:HE1	1:E:300:GLU:HB2	1.36	1.03
1:B:487:MET:HE1	1:D:463:ILE:HD11	1.06	1.03
1:D:441:MET:HE3	1:D:445:GLU:HB3	1.40	1.02
1:F:213:MET:HE3	1:H:533:ALA:HB1	1.42	1.01
1:H:441:MET:HE3	1:H:445:GLU:HB3	1.41	1.00
1:B:219:VAL:HG12	1:B:220:PRO:HD2	1.39	0.99
1:B:333:LYS:HE3	1:E:492:GLN:NE2	1.78	0.99
1:E:463:ILE:HD11	1:G:487:MET:CE	1.91	0.99
1:B:487:MET:CE	1:D:463:ILE:HD11	1.93	0.97
1:A:70:HIS:HD2	1:A:75:THR:HG23	1.30	0.97
1:F:222:GLN:HE22	1:F:225:ILE:HD11	1.26	0.97
1:A:70:HIS:HD2	1:A:75:THR:CG2	1.77	0.96
1:B:464:THR:HG23	1:B:465:LEU:HG	1.50	0.93
1:F:70:HIS:HD2	1:F:75:THR:HG22	1.31	0.93
1:F:29:PRO:O	1:F:32:ARG:CD	2.17	0.93
1:F:464:THR:HG23	1:F:465:LEU:HG	1.51	0.92
1:H:464:THR:HG23	1:H:465:LEU:HG	1.51	0.92
1:G:464:THR:HG23	1:G:465:LEU:HG	1.51	0.91
1:E:523:MET:HE2	1:H:46:LYS:HE2	1.52	0.91
1:F:219:VAL:CG1	1:F:220:PRO:HD2	2.00	0.90
1:B:30:ARG:NH1	1:B:241:ASN:O	2.05	0.89
1:B:219:VAL:CG1	1:B:220:PRO:HD2	2.01	0.89
1:A:534:MET:HA	1:A:538:VAL:HG21	1.55	0.89
1:E:523:MET:CE	1:H:46:LYS:HE2	2.02	0.89
1:D:299:ILE:O	1:D:302:GLU:HG3	1.73	0.89
1:G:382:THR:HA	1:G:401:MET:HE1	1.55	0.89
1:G:534:MET:HA	1:G:538:VAL:HG21	1.54	0.88
1:H:207:THR:O	1:H:209:LYS:NZ	2.07	0.88
1:B:534:MET:HA	1:B:538:VAL:HG21	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:382:THR:HA	1:F:401:MET:HE1	1.56	0.87
1:A:70:HIS:CD2	1:A:75:THR:CG2	2.58	0.86
1:E:103:TRP:CH2	1:G:509:GLN:OE1	2.28	0.86
1:F:534:MET:HA	1:F:538:VAL:HG21	1.54	0.86
1:G:296:LEU:O	1:G:299:ILE:HG23	1.75	0.86
1:A:70:HIS:CD2	1:A:75:THR:HG23	2.13	0.83
1:F:531:THR:HG22	1:H:209:LYS:NZ	1.93	0.83
1:G:296:LEU:O	1:G:299:ILE:CG2	2.27	0.82
1:E:533:ALA:CB	1:G:213:MET:HE3	2.11	0.81
1:G:385:ALA:CB	1:G:401:MET:HE3	2.11	0.81
1:H:120:ALA:HB3	1:H:208:LYS:HG2	1.61	0.81
1:F:70:HIS:CD2	1:F:75:THR:HG22	2.15	0.80
1:E:148:GLU:OE1	1:E:510:LYS:HE2	1.82	0.80
1:B:296:LEU:HD22	1:D:528:VAL:CG2	2.11	0.79
1:A:533:ALA:CB	1:C:213:MET:HE3	2.13	0.79
1:G:208:LYS:HE3	1:G:209:LYS:O	1.83	0.79
1:A:33:LYS:NZ	1:A:425:GLN:CD	2.40	0.79
1:E:148:GLU:OE1	1:E:510:LYS:CE	2.30	0.79
1:E:219:VAL:CG2	1:E:220:PRO:HD2	2.12	0.79
1:B:487:MET:HA	1:B:487:MET:HE2	1.65	0.79
1:F:385:ALA:CB	1:F:401:MET:HE3	2.12	0.78
1:F:233:ALA:O	1:F:237:ILE:HG22	1.82	0.78
1:F:429:TYR:HD2	1:F:431:LEU:CD2	1.97	0.78
1:C:515:THR:O	1:C:518:ASP:OD1	2.02	0.78
1:G:219:VAL:CG2	1:G:220:PRO:HD2	2.12	0.77
1:D:301:SER:O	1:D:305:LYS:HG2	1.83	0.77
1:G:487:MET:HA	1:G:487:MET:HE2	1.65	0.77
1:B:333:LYS:HE3	1:E:492:GLN:HE22	1.47	0.76
1:E:283:MET:CE	1:E:300:GLU:HB2	2.12	0.76
1:G:232:ARG:HG2	1:G:232:ARG:NH2	1.94	0.76
1:F:221:VAL:O	1:F:225:ILE:HG23	1.86	0.75
1:G:340:ASN:HB2	1:G:341:PRO:HD2	1.67	0.75
1:F:213:MET:HE3	1:H:533:ALA:CB	2.15	0.75
1:B:340:ASN:HB2	1:B:341:PRO:HD2	1.68	0.75
1:D:340:ASN:HB2	1:D:341:PRO:HD2	1.69	0.75
1:A:33:LYS:NZ	1:A:425:GLN:OE1	2.20	0.74
1:G:382:THR:HA	1:G:401:MET:CE	2.17	0.74
1:E:340:ASN:HB2	1:E:341:PRO:HD2	1.69	0.74
1:H:340:ASN:HB2	1:H:341:PRO:HD2	1.70	0.74
1:C:340:ASN:HB2	1:C:341:PRO:HD2	1.68	0.74
1:B:219:VAL:HG11	1:B:223:GLU:CD	2.12	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:LYS:HZ3	1:E:425:GLN:HA	1.51	0.74
1:F:219:VAL:HG11	1:F:223:GLU:CD	2.12	0.74
1:B:33:LYS:HZ3	1:B:425:GLN:HA	1.53	0.73
1:B:172:ASP:OD2	4:B:701:HOH:O	2.06	0.73
1:F:222:GLN:NE2	1:F:225:ILE:HD11	2.02	0.73
1:G:385:ALA:HB3	1:G:401:MET:HE3	1.69	0.73
1:A:340:ASN:HB2	1:A:341:PRO:HD2	1.69	0.73
1:B:283:MET:HE1	1:B:300:GLU:HB2	1.70	0.73
1:G:288:SER:C	1:G:289:LYS:HG2	2.13	0.73
1:F:382:THR:HA	1:F:401:MET:CE	2.18	0.73
1:G:33:LYS:HE2	4:G:740:HOH:O	1.87	0.72
1:B:219:VAL:HG12	1:B:220:PRO:CD	2.17	0.72
1:F:340:ASN:HB2	1:F:341:PRO:HD2	1.70	0.72
1:D:490:TYR:CE1	1:D:494:VAL:HG21	2.25	0.72
1:F:385:ALA:HB3	1:F:401:MET:HE3	1.71	0.72
1:G:288:SER:O	1:G:289:LYS:CG	2.37	0.72
1:A:33:LYS:HZ2	1:A:425:GLN:CD	1.97	0.71
1:A:490:TYR:CE1	1:A:494:VAL:HG21	2.25	0.71
1:D:299:ILE:HA	1:D:302:GLU:HG2	1.72	0.71
1:B:66:LEU:HD11	1:B:96:ASP:OD2	1.90	0.70
1:C:177:HIS:HD2	4:C:712:HOH:O	1.73	0.70
1:E:490:TYR:CE1	1:E:494:VAL:HG21	2.26	0.70
1:D:441:MET:HE2	1:D:446:GLN:HA	1.72	0.70
1:D:441:MET:HE2	1:D:446:GLN:N	2.06	0.70
1:F:219:VAL:HG12	1:F:220:PRO:CD	2.17	0.70
1:H:441:MET:HE2	1:H:446:GLN:N	2.06	0.70
1:H:441:MET:HE2	1:H:446:GLN:HA	1.72	0.70
1:C:490:TYR:CE1	1:C:494:VAL:HG21	2.26	0.70
1:G:66:LEU:HD11	1:G:96:ASP:OD2	1.91	0.70
1:G:148:GLU:O	1:G:152:LEU:HD13	1.91	0.70
1:E:219:VAL:CG2	1:E:223:GLU:OE2	2.40	0.70
1:D:66:LEU:HD11	1:D:96:ASP:OD2	1.91	0.69
1:E:539:THR:CG2	1:G:212:HIS:HB3	2.22	0.69
1:H:63:LEU:HD13	1:H:63:LEU:O	1.92	0.69
1:H:66:LEU:HD11	1:H:96:ASP:OD2	1.91	0.69
1:D:441:MET:HE3	1:D:445:GLU:CB	2.18	0.69
1:E:66:LEU:HD11	1:E:96:ASP:OD2	1.92	0.69
1:H:441:MET:HE2	1:H:446:GLN:CA	2.22	0.69
1:F:187:THR:HG21	1:F:231:ILE:HA	1.73	0.69
1:H:473:LEU:CD2	1:H:473:LEU:C	2.66	0.69
1:G:15:PHE:O	1:G:19:VAL:HG13	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ARG:NH1	1:D:236:ASP:OD2	2.25	0.69
1:F:531:THR:HG22	1:H:209:LYS:HZ1	1.56	0.69
1:D:441:MET:HE2	1:D:446:GLN:CA	2.22	0.69
1:F:318:ASP:O	1:F:322:ASN:ND2	2.26	0.69
1:F:342:LEU:HD21	1:F:386:VAL:CG2	2.23	0.69
1:H:441:MET:HE3	1:H:445:GLU:CB	2.18	0.69
1:C:174:ASP:OD2	1:C:177:HIS:HE1	1.75	0.68
1:D:36:ARG:NH1	1:D:236:ASP:OD1	2.25	0.68
1:F:122:TYR:HB2	1:F:126:THR:HG21	1.75	0.68
1:G:219:VAL:HG22	1:G:220:PRO:CD	2.18	0.68
1:H:473:LEU:C	1:H:473:LEU:HD22	2.18	0.68
1:G:219:VAL:HG21	1:G:223:GLU:CD	2.18	0.68
1:G:33:LYS:NZ	1:G:424:ASP:O	2.25	0.68
1:A:302:GLU:O	1:A:306:LYS:HG2	1.94	0.68
1:C:340:ASN:HB2	1:C:341:PRO:CD	2.24	0.67
1:A:33:LYS:HG3	1:A:33:LYS:O	1.93	0.67
1:B:291:ILE:HG23	1:B:295:GLU:HG3	1.75	0.67
1:G:340:ASN:HB2	1:G:341:PRO:CD	2.23	0.67
1:A:494:VAL:CG2	1:A:495:GLN:N	2.58	0.67
1:H:120:ALA:CB	1:H:208:LYS:HG2	2.25	0.67
1:B:314:GLU:O	1:B:317:ILE:HG13	1.93	0.67
1:D:36:ARG:NH1	1:D:236:ASP:CG	2.53	0.67
1:B:490:TYR:OH	1:D:433:PRO:HB3	1.95	0.67
1:C:494:VAL:CG2	1:C:495:GLN:N	2.58	0.66
1:D:340:ASN:HB2	1:D:341:PRO:CD	2.25	0.66
1:A:340:ASN:HB2	1:A:341:PRO:CD	2.24	0.66
1:E:33:LYS:O	1:E:33:LYS:HG2	1.96	0.66
1:E:103:TRP:CZ3	1:G:509:GLN:OE1	2.48	0.66
1:G:494:VAL:CG2	1:G:495:GLN:N	2.59	0.66
1:H:464:THR:CG2	1:H:465:LEU:HG	2.26	0.66
1:E:494:VAL:CG2	1:E:495:GLN:N	2.58	0.66
1:H:340:ASN:HB2	1:H:341:PRO:CD	2.25	0.66
1:B:340:ASN:HB2	1:B:341:PRO:CD	2.24	0.66
1:A:329:ASP:O	1:A:332:ILE:HG13	1.95	0.66
1:D:494:VAL:CG2	1:D:495:GLN:N	2.58	0.66
1:G:329:ASP:O	1:G:332:ILE:HG13	1.95	0.66
1:G:464:THR:CG2	1:G:465:LEU:HG	2.26	0.66
1:A:70:HIS:CD2	1:A:75:THR:HG22	2.31	0.66
1:B:150:LEU:HA	1:B:157:ARG:NH1	2.11	0.66
1:D:317:ILE:HG12	1:D:332:ILE:HD12	1.78	0.66
1:E:539:THR:OG1	1:E:542:GLN:NE2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:THR:HG23	1:B:465:LEU:CG	2.26	0.66
1:E:340:ASN:HB2	1:E:341:PRO:CD	2.25	0.66
1:E:433:PRO:HB3	1:G:490:TYR:OH	1.95	0.66
1:F:29:PRO:O	1:F:32:ARG:HG3	1.96	0.66
1:C:518:ASP:OD1	1:C:519:GLY:N	2.30	0.65
1:F:329:ASP:O	1:F:332:ILE:HG13	1.95	0.65
1:G:232:ARG:HH21	1:G:232:ARG:CG	2.00	0.65
1:B:464:THR:CG2	1:B:465:LEU:HG	2.25	0.65
1:E:103:TRP:CH2	1:G:509:GLN:CD	2.74	0.65
1:E:219:VAL:HG22	1:E:220:PRO:CD	2.18	0.65
1:E:490:TYR:OH	1:G:433:PRO:HB3	1.97	0.65
1:F:464:THR:HG23	1:F:465:LEU:CG	2.26	0.65
1:G:302:GLU:O	1:G:306:LYS:HG3	1.97	0.65
1:H:291:ILE:HG23	1:H:295:GLU:CG	2.27	0.65
1:E:498:GLU:HG2	1:E:503:VAL:HG11	1.79	0.65
1:B:433:PRO:HB3	1:D:490:TYR:OH	1.96	0.65
1:D:441:MET:CE	1:D:445:GLU:HB3	2.24	0.65
1:F:29:PRO:O	1:F:32:ARG:CG	2.45	0.65
1:F:75:THR:HG23	1:F:76:VAL:N	2.12	0.65
1:B:33:LYS:HG2	1:B:33:LYS:O	1.95	0.65
1:E:496:GLN:CD	1:G:438:ASN:ND2	2.55	0.65
1:F:46:LYS:HB3	1:F:237:ILE:HD12	1.79	0.64
1:H:329:ASP:O	1:H:332:ILE:HG13	1.96	0.64
1:F:340:ASN:HB2	1:F:341:PRO:CD	2.25	0.64
1:F:464:THR:CG2	1:F:465:LEU:HG	2.26	0.64
1:G:288:SER:O	1:G:289:LYS:HG3	1.97	0.64
1:G:128:PRO:O	1:G:131:VAL:HG22	1.97	0.64
1:E:33:LYS:NZ	1:E:425:GLN:HA	2.12	0.64
1:F:382:THR:O	1:F:386:VAL:HG13	1.96	0.64
1:H:63:LEU:HD23	1:H:168:PRO:HB2	1.80	0.64
1:B:296:LEU:HD23	1:D:528:VAL:HG21	1.76	0.64
1:C:448:THR:HG23	1:C:452:ARG:HE	1.62	0.64
1:E:460:TRP:CZ3	1:E:462:PHE:HE2	2.14	0.64
1:F:128:PRO:O	1:F:131:VAL:HG22	1.98	0.64
1:C:209:LYS:HD2	1:C:213:MET:CE	2.28	0.64
1:F:149:ARG:NH2	1:G:11:GLU:OE2	2.30	0.64
1:G:282:LEU:HG	1:G:299:ILE:HD11	1.79	0.64
1:G:464:THR:HG23	1:G:465:LEU:CG	2.27	0.64
1:E:460:TRP:CZ3	1:E:462:PHE:CE2	2.86	0.64
1:E:103:TRP:CE3	1:E:118:ASP:HB2	2.33	0.64
1:B:88:VAL:HG13	1:B:98:ILE:CD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:GLU:O	1:C:306:LYS:HG3	1.97	0.64
1:B:33:LYS:NZ	1:B:425:GLN:HA	2.12	0.63
1:D:494:VAL:HG23	1:D:495:GLN:N	2.13	0.63
1:F:383:GLN:HA	1:F:386:VAL:HG13	1.80	0.63
1:H:464:THR:HG23	1:H:465:LEU:CG	2.26	0.63
1:F:490:TYR:OH	1:H:433:PRO:HB3	1.99	0.63
1:G:209:LYS:HD2	1:G:213:MET:CE	2.28	0.63
1:D:301:SER:O	1:D:305:LYS:CG	2.46	0.63
1:F:66:LEU:HD22	1:F:66:LEU:O	1.98	0.63
1:F:209:LYS:HD2	1:F:213:MET:CE	2.28	0.63
1:E:18:GLU:OE2	1:E:51:LYS:HE2	1.99	0.63
1:B:128:PRO:O	1:B:131:VAL:HG22	1.98	0.63
1:D:503:VAL:HG12	1:D:505:VAL:HG13	1.81	0.63
1:E:303:TRP:HZ2	1:E:368:VAL:CG1	2.12	0.63
1:D:303:TRP:HZ2	1:D:368:VAL:CG1	2.12	0.62
1:E:128:PRO:O	1:E:131:VAL:HG22	1.98	0.62
1:E:494:VAL:HG23	1:E:495:GLN:N	2.13	0.62
1:E:539:THR:CG2	1:G:434:SER:HB3	2.29	0.62
1:A:490:TYR:O	1:A:494:VAL:HG22	1.99	0.62
1:D:88:VAL:HG13	1:D:98:ILE:CD1	2.28	0.62
1:E:30:ARG:NH2	1:E:243:LEU:CD2	2.62	0.62
1:F:111:THR:H	1:F:126:THR:HG22	1.64	0.62
1:H:441:MET:CE	1:H:445:GLU:HB3	2.25	0.62
1:A:88:VAL:HG13	1:A:98:ILE:CD1	2.29	0.62
1:A:494:VAL:HG23	1:A:495:GLN:N	2.13	0.62
1:C:490:TYR:O	1:C:494:VAL:HG22	1.99	0.62
1:B:283:MET:CE	1:B:300:GLU:HB2	2.30	0.62
1:E:490:TYR:O	1:E:494:VAL:HG22	2.00	0.62
1:G:494:VAL:HG23	1:G:495:GLN:N	2.14	0.62
1:H:37:ILE:O	1:H:37:ILE:CG2	2.47	0.62
1:F:538:VAL:HG23	1:H:214:ALA:HB2	1.81	0.62
1:F:303:TRP:HZ2	1:F:368:VAL:CG1	2.13	0.62
1:G:490:TYR:O	1:G:494:VAL:HG22	1.99	0.62
1:H:291:ILE:HG23	1:H:295:GLU:HG3	1.82	0.62
1:E:157:ARG:HH12	1:H:12:GLU:HG2	1.64	0.61
1:B:472:ALA:HB1	1:D:505:VAL:HG11	1.82	0.61
1:C:494:VAL:HG23	1:C:495:GLN:N	2.13	0.61
1:D:490:TYR:O	1:D:494:VAL:HG22	2.00	0.61
1:H:464:THR:HG21	3:H:603:FMT:O2	2.00	0.61
1:A:33:LYS:HZ1	1:A:425:GLN:HA	1.66	0.61
1:E:434:SER:HB3	1:G:539:THR:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:525:SER:HB2	1:E:529:THR:HG23	1.82	0.61
1:E:30:ARG:NH2	1:E:243:LEU:HD23	2.16	0.61
1:F:174:ASP:O	1:F:201:GLU:HG3	2.01	0.60
1:G:170:ILE:HD12	1:G:460:TRP:CE2	2.36	0.60
1:G:288:SER:C	1:G:289:LYS:CG	2.74	0.60
1:A:174:ASP:O	1:A:201:GLU:HG3	2.01	0.60
1:D:441:MET:CE	1:D:445:GLU:C	2.75	0.60
1:E:450:ILE:HG13	1:E:451:LYS:H	1.66	0.60
1:F:75:THR:HG23	1:F:76:VAL:H	1.66	0.60
1:C:170:ILE:HD12	1:C:460:TRP:CE2	2.37	0.60
1:F:531:THR:CG2	1:H:209:LYS:HZ1	2.14	0.60
1:F:531:THR:HG21	1:H:207:THR:HB	1.82	0.60
1:B:170:ILE:HD12	1:B:460:TRP:CE2	2.37	0.60
1:B:174:ASP:O	1:B:201:GLU:HG3	2.01	0.60
1:H:464:THR:HG21	3:H:603:FMT:C	2.31	0.60
1:E:487:MET:HE2	1:G:437:TRP:CE2	2.37	0.60
1:A:490:TYR:OH	1:C:433:PRO:HB3	2.02	0.60
1:E:170:ILE:HD12	1:E:460:TRP:CE2	2.36	0.60
1:E:189:MET:O	1:E:193:ARG:HG3	2.02	0.60
1:A:170:ILE:HD12	1:A:460:TRP:CE2	2.36	0.59
1:B:219:VAL:CG1	1:B:220:PRO:CD	2.80	0.59
1:E:174:ASP:O	1:E:201:GLU:HG3	2.02	0.59
1:D:170:ILE:HD12	1:D:460:TRP:CE2	2.37	0.59
1:H:441:MET:CE	1:H:445:GLU:C	2.74	0.59
1:G:174:ASP:O	1:G:201:GLU:HG3	2.02	0.59
1:C:174:ASP:O	1:C:201:GLU:HG3	2.02	0.59
1:H:170:ILE:HD12	1:H:460:TRP:CE2	2.37	0.59
1:E:103:TRP:HH2	1:G:509:GLN:CD	2.09	0.59
1:F:448:THR:HG23	1:F:452:ARG:HH21	1.67	0.59
1:F:170:ILE:HD12	1:F:460:TRP:CE2	2.37	0.59
1:H:174:ASP:O	1:H:201:GLU:HG3	2.01	0.59
1:A:433:PRO:HB3	1:C:490:TYR:OH	2.03	0.59
1:A:84:ASP:HB2	1:A:85:PRO:HD2	1.85	0.59
1:H:84:ASP:HB2	1:H:85:PRO:HD2	1.85	0.59
1:B:33:LYS:HZ3	1:B:425:GLN:CD	2.11	0.58
1:B:437:TRP:CE2	1:D:487:MET:HE2	2.38	0.58
1:C:174:ASP:OD1	4:C:701:HOH:O	2.16	0.58
1:F:531:THR:CG2	1:H:209:LYS:NZ	2.66	0.58
1:D:174:ASP:O	1:D:201:GLU:HG3	2.01	0.58
1:F:382:THR:O	1:F:386:VAL:CG1	2.51	0.58
1:B:219:VAL:HG11	1:B:223:GLU:CG	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLU:HA	1:B:317:ILE:HD11	1.86	0.58
1:B:525:SER:HB2	1:B:529:THR:HG23	1.83	0.58
1:F:219:VAL:CG1	1:F:220:PRO:CD	2.79	0.58
1:E:353:LEU:HG	1:E:357:LEU:HD13	1.84	0.58
1:E:523:MET:HE1	1:H:46:LYS:HE2	1.85	0.58
1:G:84:ASP:HB2	1:G:85:PRO:HD2	1.85	0.58
1:B:509:GLN:HE21	1:B:509:GLN:HA	1.67	0.58
1:E:324:ASN:CG	1:E:324:ASN:O	2.47	0.58
1:G:296:LEU:O	1:G:299:ILE:HG22	2.03	0.58
1:E:84:ASP:HB2	1:E:85:PRO:HD2	1.85	0.58
1:A:116:SER:OG	1:A:117:PRO:O	2.22	0.58
1:F:84:ASP:HB2	1:F:85:PRO:HD2	1.86	0.58
1:F:222:GLN:HE22	1:F:225:ILE:CD1	2.10	0.58
1:A:441:MET:CE	1:A:445:GLU:C	2.77	0.58
1:B:331:LEU:HD21	1:B:357:LEU:HB3	1.86	0.58
1:E:283:MET:HE1	1:E:300:GLU:CB	2.25	0.57
1:A:437:TRP:CE2	1:C:487:MET:HE2	2.38	0.57
1:E:219:VAL:HG21	1:E:223:GLU:CD	2.28	0.57
1:C:84:ASP:HB2	1:C:85:PRO:HD2	1.85	0.57
1:C:324:ASN:O	1:C:324:ASN:ND2	2.34	0.57
1:D:84:ASP:HB2	1:D:85:PRO:HD2	1.85	0.57
1:B:313:HIS:O	1:B:317:ILE:HG12	2.05	0.57
1:G:232:ARG:O	1:G:232:ARG:HD3	2.04	0.57
1:B:33:LYS:O	1:B:33:LYS:CG	2.52	0.57
1:F:433:PRO:HB3	1:H:490:TYR:OH	2.05	0.57
1:B:149:ARG:C	1:B:157:ARG:NH1	2.59	0.57
1:G:332:ILE:HD12	1:G:333:LYS:N	2.20	0.57
1:F:219:VAL:HG11	1:F:223:GLU:CG	2.35	0.57
1:F:331:LEU:HD21	1:F:357:LEU:HB3	1.85	0.57
1:B:464:THR:CG2	3:B:603:FMT:O2	2.44	0.56
1:G:33:LYS:NZ	1:G:424:ASP:C	2.64	0.56
1:H:292:TYR:CD1	1:H:292:TYR:C	2.83	0.56
1:A:487:MET:HE2	1:C:437:TRP:CE2	2.40	0.56
1:B:84:ASP:HB2	1:B:85:PRO:HD2	1.86	0.56
1:D:314:GLU:O	1:D:317:ILE:HG22	2.05	0.56
1:E:539:THR:HG22	1:G:212:HIS:HB3	1.86	0.56
1:E:378:TYR:OH	1:E:388:ARG:NH1	2.38	0.56
1:F:6:ILE:HG12	1:G:162:TYR:HB3	1.88	0.56
1:H:332:ILE:HD12	1:H:333:LYS:N	2.21	0.56
1:D:299:ILE:O	1:D:302:GLU:CG	2.51	0.56
4:A:712:HOH:O	1:C:544:LYS:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:LYS:O	1:E:33:LYS:CG	2.53	0.56
1:A:332:ILE:HD12	1:A:333:LYS:N	2.21	0.56
1:B:314:GLU:HA	1:B:317:ILE:CG1	2.36	0.55
1:F:332:ILE:HD12	1:F:333:LYS:N	2.20	0.55
1:G:444:ASP:OD1	1:G:444:ASP:N	2.40	0.55
1:G:464:THR:HG21	3:G:603:FMT:O2	2.06	0.55
1:B:333:LYS:HE3	1:E:492:GLN:CD	2.31	0.55
1:E:175:THR:HG23	1:E:175:THR:O	2.06	0.55
1:C:282:LEU:O	1:C:285:GLU:HG2	2.06	0.55
1:D:31:TRP:CD2	1:D:36:ARG:NH2	2.74	0.55
1:A:262:HIS:CE1	1:A:263:ARG:HG3	2.42	0.55
1:E:539:THR:HG21	1:G:434:SER:HB3	1.89	0.55
1:E:104:GLN:O	1:E:108:THR:HB	2.05	0.55
1:E:261:ASP:OD1	1:E:263:ARG:HD2	2.07	0.55
1:E:393:ALA:N	1:E:394:PRO:CD	2.70	0.55
1:E:434:SER:HB3	1:G:539:THR:HG21	1.87	0.55
1:F:541:ASP:OD1	1:F:541:ASP:N	2.39	0.55
1:H:63:LEU:HD11	1:H:67:LEU:CD1	2.37	0.55
1:A:33:LYS:NZ	1:A:425:GLN:HA	2.21	0.55
1:C:393:ALA:N	1:C:394:PRO:CD	2.70	0.54
1:H:63:LEU:HD11	1:H:67:LEU:HD11	1.89	0.54
1:A:393:ALA:N	1:A:394:PRO:CD	2.70	0.54
1:A:88:VAL:HG13	1:A:98:ILE:HD13	1.90	0.54
1:E:33:LYS:NZ	1:E:425:GLN:CD	2.66	0.54
1:G:393:ALA:N	1:G:394:PRO:CD	2.70	0.54
1:B:30:ARG:CZ	1:B:31:TRP:CZ3	2.90	0.54
1:B:88:VAL:HG13	1:B:98:ILE:HD13	1.89	0.54
1:E:33:LYS:HZ3	1:E:425:GLN:CD	2.16	0.54
1:F:234:SER:O	1:F:237:ILE:HG23	2.07	0.54
1:G:208:LYS:CE	1:G:209:LYS:O	2.56	0.54
1:D:393:ALA:N	1:D:394:PRO:CD	2.71	0.54
1:D:88:VAL:HG13	1:D:98:ILE:HD13	1.89	0.54
1:H:444:ASP:N	1:H:444:ASP:OD1	2.40	0.54
1:B:33:LYS:NZ	1:B:425:GLN:CD	2.65	0.54
1:C:209:LYS:HD2	1:C:213:MET:HE2	1.90	0.54
1:E:93:LYS:NZ	1:E:504:GLU:OE1	2.35	0.54
1:H:37:ILE:O	1:H:37:ILE:HG22	2.07	0.54
1:A:485:ILE:HG12	1:A:488:LYS:HB3	1.90	0.53
1:F:222:GLN:NE2	1:F:225:ILE:CD1	2.71	0.53
1:F:393:ALA:N	1:F:394:PRO:CD	2.70	0.53
1:G:482:TYR:HE1	1:G:487:MET:CE	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:THR:HA	1:D:85:PRO:HG2	1.89	0.53
1:B:393:ALA:N	1:B:394:PRO:CD	2.70	0.53
1:E:175:THR:O	1:E:175:THR:CG2	2.57	0.53
1:E:525:SER:CB	1:E:529:THR:CG2	2.87	0.53
1:H:393:ALA:N	1:H:394:PRO:CD	2.71	0.53
1:A:444:ASP:OD1	1:A:444:ASP:N	2.40	0.53
1:B:30:ARG:HH12	1:B:241:ASN:C	2.15	0.53
1:E:444:ASP:N	1:E:444:ASP:OD1	2.40	0.53
1:H:63:LEU:CD1	1:H:63:LEU:C	2.82	0.53
1:G:128:PRO:O	1:G:131:VAL:CG2	2.57	0.53
1:D:503:VAL:CG1	1:D:505:VAL:HG13	2.38	0.53
1:E:103:TRP:CD1	1:E:103:TRP:C	2.86	0.53
1:F:433:PRO:HG2	1:F:465:LEU:HB2	1.91	0.53
1:C:6:ILE:HG13	1:C:7:ASP:N	2.24	0.53
1:E:219:VAL:HG21	1:E:223:GLU:OE2	2.07	0.53
1:H:441:MET:CE	1:H:446:GLN:N	2.71	0.53
1:E:433:PRO:HG2	1:E:465:LEU:HB2	1.91	0.53
1:F:6:ILE:HG12	1:G:162:TYR:CB	2.38	0.53
1:F:487:MET:HE2	1:H:437:TRP:CE2	2.44	0.53
1:D:433:PRO:HG2	1:D:465:LEU:HB2	1.91	0.53
1:G:103:TRP:CD1	1:G:118:ASP:HB2	2.44	0.53
1:B:482:TYR:HE1	1:B:487:MET:CE	2.22	0.52
1:F:70:HIS:HD2	1:F:75:THR:CG2	2.11	0.52
1:A:441:MET:HE2	1:A:446:GLN:N	2.24	0.52
1:B:433:PRO:HG2	1:B:465:LEU:HB2	1.91	0.52
1:H:63:LEU:CD1	1:H:67:LEU:CD1	2.86	0.52
1:B:219:VAL:CG1	1:B:223:GLU:CD	2.82	0.52
1:E:170:ILE:HD12	1:E:460:TRP:CZ2	2.45	0.52
1:E:496:GLN:OE1	1:G:438:ASN:ND2	2.43	0.52
1:F:58:GLN:O	1:F:61:ASP:OD1	2.28	0.52
1:F:128:PRO:O	1:F:193:ARG:HD3	2.10	0.52
1:F:203:GLN:HE22	1:F:209:LYS:H	1.56	0.52
1:A:103:TRP:CD1	1:A:118:ASP:HB2	2.45	0.52
1:A:433:PRO:HG2	1:A:465:LEU:HB2	1.91	0.52
1:C:317:ILE:HG12	1:C:332:ILE:HG23	1.90	0.52
1:C:448:THR:HG23	1:C:452:ARG:NE	2.24	0.52
1:E:128:PRO:O	1:E:131:VAL:CG2	2.57	0.52
1:F:85:PRO:HG2	1:H:108:THR:HA	1.92	0.52
1:F:431:LEU:HD23	1:F:431:LEU:N	2.24	0.52
1:B:85:PRO:HG2	1:D:108:THR:HA	1.90	0.52
1:C:170:ILE:HD12	1:C:460:TRP:CZ2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:THR:CG2	1:F:76:VAL:N	2.73	0.52
1:F:276:ALA:CA	1:F:306:LYS:NZ	2.60	0.52
1:G:433:PRO:HG2	1:G:465:LEU:HB2	1.91	0.52
1:H:6:ILE:HG13	1:H:7:ASP:N	2.24	0.52
1:A:33:LYS:HE2	4:A:715:HOH:O	2.10	0.52
1:B:393:ALA:HB1	1:B:425:GLN:HE21	1.75	0.52
1:B:525:SER:CB	1:B:529:THR:CG2	2.88	0.52
1:F:108:THR:HA	1:H:85:PRO:HG2	1.92	0.52
1:F:436:ASN:HD22	1:F:437:TRP:N	2.06	0.52
1:B:30:ARG:NH1	1:B:241:ASN:C	2.67	0.52
1:C:433:PRO:HG2	1:C:465:LEU:HB2	1.91	0.52
1:F:103:TRP:CD1	1:F:118:ASP:HB2	2.45	0.52
1:G:6:ILE:HG13	1:G:7:ASP:N	2.24	0.52
1:G:209:LYS:HD2	1:G:213:MET:HE2	1.90	0.52
1:H:103:TRP:CD1	1:H:118:ASP:HB2	2.45	0.52
1:H:433:PRO:HG2	1:H:465:LEU:HB2	1.91	0.52
1:B:88:VAL:HG21	1:B:134:LEU:HB3	1.92	0.52
1:C:448:THR:HG23	1:C:452:ARG:HH21	1.74	0.52
1:D:103:TRP:CD1	1:D:118:ASP:HB2	2.44	0.52
1:D:441:MET:CE	1:D:446:GLN:N	2.71	0.52
1:F:209:LYS:HD2	1:F:213:MET:HE2	1.91	0.52
1:B:170:ILE:HD12	1:B:460:TRP:CZ2	2.45	0.51
1:A:170:ILE:HD12	1:A:460:TRP:CZ2	2.45	0.51
1:E:528:VAL:HG23	1:G:372:ARG:NH2	2.25	0.51
1:A:9:GLN:HE21	1:A:9:GLN:HA	1.75	0.51
1:F:170:ILE:HD12	1:F:460:TRP:CZ2	2.45	0.51
1:F:429:TYR:CD2	1:F:431:LEU:CD2	2.86	0.51
1:B:103:TRP:CD1	1:B:118:ASP:HB2	2.45	0.51
1:C:103:TRP:CD1	1:C:118:ASP:HB2	2.45	0.51
1:G:170:ILE:HD12	1:G:460:TRP:CZ2	2.45	0.51
1:D:207:THR:O	1:D:209:LYS:HD3	2.11	0.51
1:F:128:PRO:O	1:F:131:VAL:CG2	2.57	0.51
1:H:473:LEU:CD2	1:H:473:LEU:O	2.59	0.51
1:B:128:PRO:O	1:B:131:VAL:CG2	2.58	0.51
1:F:251:GLU:CG	1:F:401:MET:HE2	2.40	0.51
1:G:490:TYR:CE2	1:G:494:VAL:HG21	2.46	0.51
1:B:199:HIS:CB	1:B:245:VAL:HB	2.41	0.51
1:B:393:ALA:CB	1:B:425:GLN:HE21	2.24	0.51
1:E:103:TRP:O	1:E:106:SER:OG	2.24	0.51
1:A:88:VAL:HG21	1:A:134:LEU:HB3	1.93	0.51
1:B:30:ARG:HH11	1:B:241:ASN:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:LYS:O	1:C:332:ILE:HG12	2.11	0.51
1:H:63:LEU:HD13	1:H:63:LEU:C	2.35	0.51
1:D:88:VAL:HG21	1:D:134:LEU:HB3	1.93	0.51
1:F:199:HIS:CB	1:F:245:VAL:HB	2.41	0.51
1:D:170:ILE:HD12	1:D:460:TRP:CZ2	2.46	0.50
1:D:490:TYR:CD1	1:D:494:VAL:HG21	2.46	0.50
1:A:441:MET:CE	1:A:446:GLN:N	2.74	0.50
1:G:199:HIS:CB	1:G:245:VAL:HB	2.42	0.50
1:H:199:HIS:CB	1:H:245:VAL:HB	2.41	0.50
1:A:112:SER:O	1:A:113:ASN:HB2	2.11	0.50
1:C:127:VAL:HB	1:C:128:PRO:HD3	1.94	0.50
1:H:170:ILE:HD12	1:H:460:TRP:CZ2	2.46	0.50
1:B:314:GLU:HA	1:B:317:ILE:HG12	1.94	0.50
1:D:199:HIS:CB	1:D:245:VAL:HB	2.41	0.50
1:G:251:GLU:CG	1:G:401:MET:HE2	2.40	0.50
1:E:359:GLY:CA	1:E:360:LYS:HD2	2.41	0.50
1:G:152:LEU:N	1:G:152:LEU:CD1	2.74	0.50
1:H:112:SER:O	1:H:113:ASN:HB2	2.12	0.50
1:B:112:SER:O	1:B:113:ASN:HB2	2.11	0.50
1:B:133:HIS:CE1	4:B:730:HOH:O	2.65	0.50
1:E:127:VAL:HB	1:E:128:PRO:HD3	1.94	0.50
1:E:490:TYR:CD1	1:E:494:VAL:HG21	2.47	0.50
1:F:266:TYR:CE2	1:F:340:ASN:HA	2.47	0.50
1:B:285:GLU:O	1:B:289:LYS:HG2	2.11	0.49
1:C:199:HIS:CB	1:C:245:VAL:HB	2.42	0.49
1:E:393:ALA:CB	1:E:425:GLN:HE21	2.25	0.49
1:A:127:VAL:HB	1:A:128:PRO:HD3	1.94	0.49
1:C:112:SER:O	1:C:113:ASN:HB2	2.12	0.49
1:E:199:HIS:CB	1:E:245:VAL:HB	2.42	0.49
1:F:342:LEU:CD2	1:F:386:VAL:CG2	2.90	0.49
1:A:88:VAL:HG11	1:A:138:GLN:CG	2.42	0.49
1:A:199:HIS:CB	1:A:245:VAL:HB	2.42	0.49
1:D:328:LYS:O	1:D:332:ILE:HG12	2.11	0.49
1:E:112:SER:O	1:E:113:ASN:HB2	2.13	0.49
1:F:436:ASN:HD22	1:F:436:ASN:C	2.19	0.49
1:A:490:TYR:CD1	1:A:494:VAL:HG21	2.47	0.49
1:C:174:ASP:OD2	1:C:177:HIS:CE1	2.61	0.49
1:C:490:TYR:CD1	1:C:494:VAL:HG21	2.47	0.49
1:E:450:ILE:HG13	1:E:451:LYS:N	2.27	0.49
1:F:531:THR:HG22	1:H:209:LYS:HZ3	1.75	0.49
1:B:88:VAL:HG11	1:B:138:GLN:CG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:TYR:CE2	1:A:340:ASN:HA	2.48	0.49
1:D:88:VAL:HG11	1:D:138:GLN:CG	2.43	0.49
1:E:393:ALA:HB1	1:E:425:GLN:HE21	1.77	0.49
1:F:112:SER:O	1:F:113:ASN:HB2	2.13	0.49
1:F:127:VAL:HB	1:F:128:PRO:HD3	1.95	0.49
1:H:63:LEU:HD12	1:H:243:LEU:HD22	1.95	0.49
1:E:219:VAL:HG22	1:E:223:GLU:OE2	2.12	0.49
1:E:462:PHE:HD1	1:E:462:PHE:O	1.96	0.49
1:F:219:VAL:CG1	1:F:223:GLU:CD	2.83	0.49
1:B:127:VAL:HB	1:B:128:PRO:HD3	1.95	0.48
1:E:462:PHE:O	1:E:462:PHE:CD1	2.66	0.48
1:A:496:GLN:O	1:A:500:GLU:HG3	2.13	0.48
1:B:133:HIS:CE1	1:D:108:THR:O	2.66	0.48
1:D:112:SER:O	1:D:113:ASN:HB2	2.12	0.48
1:E:219:VAL:O	1:E:388:ARG:NH2	2.45	0.48
1:C:172:ASP:OD2	4:C:702:HOH:O	2.20	0.48
1:E:498:GLU:O	1:E:503:VAL:HG12	2.12	0.48
1:F:133:HIS:CE1	1:H:108:THR:O	2.67	0.48
1:H:63:LEU:CD1	1:H:67:LEU:HD12	2.43	0.48
1:A:448:THR:OG1	1:A:452:ARG:NH1	2.47	0.48
1:B:314:GLU:HA	1:B:317:ILE:CD1	2.43	0.48
1:H:127:VAL:HB	1:H:128:PRO:HD3	1.95	0.48
1:D:170:ILE:HA	1:D:197:GLY:O	2.14	0.48
1:F:496:GLN:O	1:F:500:GLU:HG3	2.13	0.48
1:A:1:MET:N	1:A:2:PRO:CD	2.77	0.48
1:G:112:SER:O	1:G:113:ASN:HB2	2.12	0.48
1:D:305:LYS:HG2	1:D:305:LYS:H	1.51	0.48
1:G:208:LYS:HD3	1:G:208:LYS:C	2.38	0.48
1:G:400:TRP:CD1	1:G:400:TRP:C	2.92	0.48
1:H:400:TRP:CD1	1:H:400:TRP:C	2.92	0.48
1:G:283:MET:CE	1:G:300:GLU:HB2	2.44	0.48
1:G:487:MET:CE	1:G:487:MET:HA	2.42	0.48
1:H:473:LEU:HD22	1:H:473:LEU:O	2.14	0.48
1:A:70:HIS:HD2	1:A:75:THR:HG22	1.63	0.47
1:C:170:ILE:HA	1:C:197:GLY:O	2.14	0.47
1:F:170:ILE:HA	1:F:197:GLY:O	2.14	0.47
1:G:318:ASP:O	1:G:321:LYS:O	2.32	0.47
1:F:71:ASP:O	1:F:74:LYS:HD3	2.14	0.47
1:G:127:VAL:HB	1:G:128:PRO:HD3	1.95	0.47
1:A:496:GLN:HG2	1:C:438:ASN:ND2	2.30	0.47
1:A:538:VAL:HG22	1:C:213:MET:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:TRP:CD1	1:C:400:TRP:C	2.91	0.47
1:D:127:VAL:HB	1:D:128:PRO:HD3	1.95	0.47
1:F:437:TRP:CE2	1:H:487:MET:HE2	2.49	0.47
1:B:33:LYS:NZ	1:B:425:GLN:CA	2.77	0.47
1:C:121:ASP:OD2	1:D:181:THR:HG22	2.14	0.47
1:C:121:ASP:OD2	1:D:181:THR:CG2	2.63	0.47
1:G:103:TRP:O	1:G:106:SER:OG	2.23	0.47
1:A:283:MET:CE	1:A:300:GLU:HB2	2.44	0.47
1:B:448:THR:OG1	1:B:452:ARG:NH1	2.48	0.47
1:C:283:MET:CE	1:C:300:GLU:HB2	2.44	0.47
1:D:400:TRP:CD1	1:D:400:TRP:C	2.92	0.47
1:D:444:ASP:OD1	1:D:444:ASP:N	2.47	0.47
1:H:32:ARG:NH2	1:H:68:GLU:OE2	2.48	0.47
1:A:170:ILE:HA	1:A:197:GLY:O	2.15	0.47
1:E:342:LEU:N	1:E:342:LEU:HD12	2.30	0.47
1:F:122:TYR:CD1	1:F:126:THR:OG1	2.57	0.47
1:F:400:TRP:CD1	1:F:400:TRP:C	2.92	0.47
1:G:170:ILE:HA	1:G:197:GLY:O	2.14	0.47
1:H:170:ILE:HA	1:H:197:GLY:O	2.14	0.47
1:B:170:ILE:HA	1:B:197:GLY:O	2.14	0.47
1:E:318:ASP:O	1:E:321:LYS:O	2.33	0.47
1:F:303:TRP:O	1:F:306:LYS:HG3	2.14	0.47
1:C:444:ASP:N	1:C:444:ASP:OD1	2.47	0.47
1:E:6:ILE:HD11	1:H:149:ARG:NH2	2.30	0.47
1:B:400:TRP:C	1:B:400:TRP:CD1	2.93	0.46
1:D:314:GLU:C	1:D:317:ILE:HG22	2.40	0.46
1:E:289:LYS:HD2	1:E:289:LYS:HA	1.60	0.46
1:F:538:VAL:HG22	1:H:213:MET:HA	1.97	0.46
1:G:482:TYR:CE1	1:G:487:MET:CE	2.98	0.46
1:E:33:LYS:NZ	1:E:425:GLN:HB2	2.30	0.46
1:F:385:ALA:HB2	1:F:401:MET:HE3	1.95	0.46
1:B:219:VAL:CG1	1:B:223:GLU:OE1	2.63	0.46
1:C:51:LYS:HE2	4:C:705:HOH:O	2.14	0.46
1:D:302:GLU:HG3	1:D:303:TRP:N	2.30	0.46
1:D:448:THR:OG1	1:D:452:ARG:NH1	2.48	0.46
1:F:149:ARG:NH2	1:F:162:TYR:CD1	2.84	0.46
1:F:219:VAL:CG1	1:F:223:GLU:OE1	2.64	0.46
1:F:283:MET:CE	1:F:300:GLU:HB2	2.45	0.46
1:F:496:GLN:HG2	1:H:438:ASN:ND2	2.30	0.46
1:A:332:ILE:HD12	1:A:332:ILE:C	2.41	0.46
1:D:75:THR:OG1	1:D:76:VAL:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:MET:CE	1:D:300:GLU:HB2	2.45	0.46
1:E:170:ILE:HA	1:E:197:GLY:O	2.15	0.46
1:H:332:ILE:HD12	1:H:332:ILE:C	2.41	0.46
1:D:266:TYR:CE2	1:D:340:ASN:HA	2.50	0.46
1:A:441:MET:CE	1:A:445:GLU:HB3	2.25	0.46
1:B:33:LYS:NZ	1:B:425:GLN:HB2	2.30	0.46
1:B:78:PHE:HE2	1:D:483:SER:HA	1.81	0.46
1:C:88:VAL:HG11	1:C:134:LEU:HB3	1.98	0.46
1:D:210:CYS:SG	3:D:603:FMT:O1	2.74	0.46
1:F:448:THR:HG23	1:F:452:ARG:CD	2.45	0.46
1:B:33:LYS:NZ	1:B:425:GLN:CB	2.79	0.46
1:B:509:GLN:NE2	1:D:213:MET:HE3	2.31	0.46
1:F:88:VAL:HG11	1:F:134:LEU:HB3	1.98	0.46
1:F:66:LEU:HD11	1:F:96:ASP:OD2	2.15	0.46
1:B:219:VAL:HG11	1:B:223:GLU:HG2	1.97	0.46
1:B:342:LEU:HD12	1:B:342:LEU:N	2.31	0.46
1:B:487:MET:HE1	1:D:463:ILE:CG1	2.46	0.46
1:E:400:TRP:CD1	1:E:400:TRP:C	2.92	0.46
1:E:523:MET:HE1	1:H:46:LYS:HG2	1.98	0.46
1:F:342:LEU:HD21	1:F:386:VAL:HG21	1.96	0.46
1:A:319:GLU:OE1	1:A:360:LYS:HE2	2.16	0.46
1:E:32:ARG:NH2	1:E:68:GLU:OE2	2.49	0.46
1:E:33:LYS:NZ	1:E:425:GLN:CA	2.77	0.46
1:E:496:GLN:CB	1:E:497:PRO:HD3	2.46	0.46
1:G:88:VAL:HG11	1:G:134:LEU:HB3	1.98	0.46
1:H:283:MET:CE	1:H:300:GLU:HB2	2.45	0.46
1:A:88:VAL:HG11	1:A:138:GLN:HG3	1.99	0.45
1:B:78:PHE:CE2	1:D:483:SER:HA	2.51	0.45
1:B:482:TYR:CE1	1:B:487:MET:CE	2.98	0.45
1:D:160:THR:HA	1:D:161:PRO:HD3	1.87	0.45
1:D:302:GLU:HG3	1:D:303:TRP:H	1.81	0.45
1:F:74:LYS:NZ	4:F:701:HOH:O	2.49	0.45
1:H:75:THR:OG1	1:H:76:VAL:N	2.49	0.45
1:F:5:PRO:C	1:F:6:ILE:HG13	2.39	0.45
1:A:496:GLN:CB	1:A:497:PRO:HD3	2.46	0.45
1:E:33:LYS:NZ	1:E:425:GLN:CB	2.79	0.45
1:E:543:PHE:C	1:E:544:LYS:HG3	2.42	0.45
1:F:332:ILE:HD12	1:F:332:ILE:C	2.40	0.45
1:A:32:ARG:NH2	1:A:68:GLU:OE2	2.50	0.45
1:B:75:THR:OG1	1:B:76:VAL:N	2.49	0.45
1:F:276:ALA:CB	1:F:306:LYS:HE3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:539:THR:OG1	1:G:542:GLN:OE1	2.34	0.45
1:C:496:GLN:CB	1:C:497:PRO:HD3	2.47	0.45
1:E:88:VAL:HG11	1:E:134:LEU:HB3	1.98	0.45
1:F:219:VAL:HG11	1:F:223:GLU:HG2	1.98	0.45
1:F:283:MET:HE2	1:F:300:GLU:OE2	2.16	0.45
1:G:219:VAL:CG2	1:G:223:GLU:CD	2.87	0.45
1:G:496:GLN:CB	1:G:497:PRO:HD3	2.47	0.45
1:A:160:THR:HA	1:A:161:PRO:HD3	1.87	0.45
1:G:449:TYR:CE2	1:G:453:LEU:HD11	2.51	0.45
1:B:292:TYR:O	1:B:295:GLU:HG2	2.16	0.45
1:B:449:TYR:CE2	1:B:453:LEU:HD11	2.52	0.45
1:G:332:ILE:HD12	1:G:332:ILE:C	2.41	0.45
1:H:88:VAL:HG11	1:H:134:LEU:HB3	1.98	0.45
1:A:145:GLN:NE2	1:A:163:ILE:O	2.48	0.45
1:A:400:TRP:CD1	1:A:400:TRP:C	2.92	0.45
1:A:449:TYR:CE2	1:A:453:LEU:HD11	2.51	0.45
1:C:283:MET:HE2	1:C:300:GLU:HB2	1.99	0.45
1:D:449:TYR:CE2	1:D:453:LEU:HD11	2.52	0.45
1:F:449:TYR:CE2	1:F:453:LEU:HD11	2.52	0.45
1:B:525:SER:HB2	1:B:529:THR:CG2	2.47	0.45
1:C:448:THR:HG23	1:C:452:ARG:NH2	2.31	0.45
1:D:88:VAL:HG11	1:D:138:GLN:HG3	1.99	0.45
1:D:283:MET:HE2	1:D:300:GLU:OE2	2.17	0.45
1:G:283:MET:HE2	1:G:300:GLU:OE2	2.17	0.45
1:A:66:LEU:HD11	1:A:96:ASP:OD2	2.16	0.44
1:B:157:ARG:HH11	1:B:157:ARG:CG	2.30	0.44
1:G:232:ARG:NH2	1:G:232:ARG:CG	2.67	0.44
1:C:449:TYR:CE2	1:C:453:LEU:HD11	2.52	0.44
1:E:430:ASN:HA	1:E:462:PHE:CE1	2.52	0.44
1:G:145:GLN:NE2	1:G:163:ILE:O	2.49	0.44
1:A:33:LYS:HZ1	1:A:425:GLN:CD	2.22	0.44
1:B:88:VAL:HG11	1:B:138:GLN:HG3	1.99	0.44
1:B:108:THR:O	1:D:133:HIS:NE2	2.48	0.44
1:H:449:TYR:CE2	1:H:453:LEU:HD11	2.52	0.44
1:A:283:MET:HE2	1:A:300:GLU:OE2	2.17	0.44
1:D:496:GLN:CB	1:D:497:PRO:HD3	2.47	0.44
1:H:496:GLN:CB	1:H:497:PRO:HD3	2.46	0.44
1:B:496:GLN:CB	1:B:497:PRO:HD3	2.47	0.44
1:E:449:TYR:CE2	1:E:453:LEU:HD11	2.51	0.44
1:E:539:THR:HG23	1:E:539:THR:O	2.17	0.44
1:H:283:MET:HE2	1:H:300:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:THR:O	1:B:209:LYS:HE2	2.18	0.44
1:C:283:MET:HE2	1:C:300:GLU:OE2	2.18	0.44
1:H:145:GLN:NE2	1:H:163:ILE:O	2.48	0.44
1:E:460:TRP:CH2	1:E:462:PHE:CD2	3.05	0.44
1:H:199:HIS:HB3	1:H:245:VAL:HB	2.00	0.44
1:A:366:TRP:CD1	1:A:366:TRP:C	2.96	0.44
1:D:145:GLN:NE2	1:D:163:ILE:O	2.48	0.44
1:F:145:GLN:NE2	1:F:163:ILE:O	2.50	0.44
1:G:152:LEU:HD13	1:G:152:LEU:N	2.32	0.44
1:H:73:ASP:HB2	1:H:75:THR:HG22	2.00	0.44
1:F:496:GLN:CB	1:F:497:PRO:HD3	2.47	0.44
1:F:70:HIS:CD2	1:F:75:THR:CG2	2.95	0.43
1:C:313:HIS:HE1	4:C:752:HOH:O	2.01	0.43
1:D:283:MET:HE2	1:D:300:GLU:HB2	2.00	0.43
1:F:283:MET:HE2	1:F:300:GLU:HB2	2.00	0.43
1:A:212:HIS:HB3	1:C:539:THR:CG2	2.48	0.43
1:A:327:ASN:HD22	1:A:327:ASN:HA	1.58	0.43
1:B:468:LEU:HD12	1:D:86:ILE:CD1	2.48	0.43
1:E:70:HIS:CE1	1:E:76:VAL:C	2.96	0.43
1:E:445:GLU:O	1:E:452:ARG:NH2	2.51	0.43
1:F:32:ARG:NH2	1:F:68:GLU:OE2	2.51	0.43
1:A:487:MET:HE2	1:C:437:TRP:CD2	2.54	0.43
1:E:199:HIS:HB3	1:E:245:VAL:HB	2.01	0.43
1:H:326:SER:O	1:H:327:ASN:C	2.61	0.43
1:A:1:MET:HB2	1:A:2:PRO:HD3	2.00	0.43
1:B:61:ASP:OD1	1:B:241:ASN:ND2	2.44	0.43
1:B:468:LEU:HD12	1:D:86:ILE:HD11	2.01	0.43
1:E:160:THR:HA	1:E:161:PRO:HD3	1.87	0.43
1:G:19:VAL:CG2	1:G:20:ALA:N	2.82	0.43
1:A:199:HIS:HB3	1:A:245:VAL:HB	2.01	0.43
1:A:283:MET:HE2	1:A:300:GLU:HB2	1.99	0.43
1:A:441:MET:HE3	1:A:445:GLU:CB	2.27	0.43
1:B:482:TYR:HE1	1:B:487:MET:HE3	1.84	0.43
1:C:207:THR:O	1:C:209:LYS:HE2	2.18	0.43
1:E:353:LEU:O	1:E:357:LEU:CD1	2.67	0.43
1:E:366:TRP:C	1:E:366:TRP:CD1	2.96	0.43
1:F:207:THR:O	1:F:209:LYS:HE2	2.18	0.43
1:F:224:HIS:HD2	1:F:227:ARG:HD2	1.84	0.43
1:G:124:MET:HE1	1:H:121:ASP:O	2.18	0.43
1:H:224:HIS:HD2	1:H:227:ARG:HD2	1.84	0.43
1:C:445:GLU:O	1:C:452:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:HIS:HB3	1:D:245:VAL:HB	2.00	0.43
1:E:212:HIS:HB3	1:G:539:THR:CG2	2.49	0.43
1:F:187:THR:CG2	1:F:231:ILE:HG12	2.48	0.43
1:G:207:THR:O	1:G:209:LYS:HE2	2.18	0.43
1:E:213:MET:HE3	1:G:509:GLN:NE2	2.34	0.43
1:E:224:HIS:HD2	1:E:227:ARG:HD2	1.83	0.43
1:G:224:HIS:HD2	1:G:227:ARG:HD2	1.83	0.43
1:G:283:MET:HE2	1:G:300:GLU:HB2	2.00	0.43
1:E:539:THR:HG22	1:G:212:HIS:CB	2.48	0.43
1:G:482:TYR:HE1	1:G:487:MET:HE3	1.83	0.43
1:B:366:TRP:CD1	1:B:366:TRP:C	2.97	0.43
1:B:438:ASN:ND2	1:D:496:GLN:HG2	2.34	0.43
1:E:207:THR:O	1:E:209:LYS:HE2	2.18	0.43
1:E:539:THR:CG2	1:G:212:HIS:CB	2.96	0.43
1:G:199:HIS:HB3	1:G:245:VAL:HB	2.00	0.43
1:G:251:GLU:HB2	1:G:401:MET:HE2	2.01	0.43
1:A:207:THR:O	1:A:209:LYS:HE2	2.19	0.42
1:B:86:ILE:CD1	1:D:468:LEU:HD12	2.49	0.42
1:B:199:HIS:HB3	1:B:245:VAL:HB	2.00	0.42
1:B:525:SER:CB	1:B:529:THR:HG23	2.48	0.42
1:F:539:THR:CG2	1:H:212:HIS:HB3	2.49	0.42
1:G:288:SER:O	1:G:289:LYS:HG2	2.11	0.42
1:A:124:MET:HE1	1:B:121:ASP:O	2.20	0.42
1:F:285:GLU:O	1:F:289:LYS:HG3	2.19	0.42
1:H:283:MET:HE2	1:H:300:GLU:HB2	2.00	0.42
1:D:79:THR:O	1:D:462:PHE:HA	2.20	0.42
1:E:213:MET:HA	1:G:538:VAL:HG22	2.01	0.42
1:E:539:THR:HG21	1:G:212:HIS:HB3	1.98	0.42
1:G:366:TRP:CD1	1:G:366:TRP:C	2.96	0.42
1:G:445:GLU:O	1:G:452:ARG:NH2	2.52	0.42
1:B:326:SER:O	1:B:327:ASN:C	2.62	0.42
1:F:199:HIS:HB3	1:F:245:VAL:HB	2.00	0.42
1:G:219:VAL:CG2	1:G:220:PRO:CD	2.90	0.42
1:G:219:VAL:CG2	1:G:223:GLU:OE1	2.68	0.42
1:A:78:PHE:HE2	1:C:483:SER:HA	1.84	0.42
1:C:366:TRP:CD1	1:C:366:TRP:C	2.98	0.42
1:D:73:ASP:HB2	1:D:75:THR:HG22	2.02	0.42
1:A:438:ASN:ND2	1:C:496:GLN:HG2	2.34	0.42
1:B:73:ASP:HB2	1:B:75:THR:HG22	2.00	0.42
1:B:219:VAL:HG13	1:B:220:PRO:HD2	1.96	0.42
1:C:127:VAL:N	1:C:128:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:THR:O	1:G:462:PHE:HA	2.20	0.42
1:B:224:HIS:HD2	1:B:227:ARG:HD2	1.84	0.42
1:B:496:GLN:HG2	1:D:438:ASN:ND2	2.35	0.42
1:E:525:SER:HB2	1:E:529:THR:CG2	2.46	0.42
1:G:539:THR:O	1:G:539:THR:HG23	2.18	0.42
1:A:224:HIS:HD2	1:A:227:ARG:HD2	1.84	0.42
1:D:224:HIS:HD2	1:D:227:ARG:HD2	1.84	0.42
1:D:314:GLU:HA	1:D:317:ILE:HG22	2.02	0.42
1:E:259:THR:HG22	1:E:268:ILE:HD13	2.01	0.42
1:F:326:SER:O	1:F:327:ASN:C	2.62	0.42
1:G:160:THR:HA	1:G:161:PRO:HD3	1.87	0.42
1:G:188:LYS:NZ	1:G:192:GLU:OE2	2.52	0.42
1:A:517:ILE:HD13	1:A:520:LEU:HD12	2.02	0.42
1:E:79:THR:O	1:E:462:PHE:HA	2.20	0.42
1:E:127:VAL:N	1:E:128:PRO:CD	2.83	0.42
1:D:127:VAL:N	1:D:128:PRO:CD	2.83	0.42
1:D:327:ASN:HD22	1:D:327:ASN:HA	1.59	0.42
1:D:366:TRP:CD1	1:D:366:TRP:C	2.98	0.42
1:E:261:ASP:OD1	1:E:263:ARG:CD	2.68	0.42
1:F:259:THR:HG22	1:F:268:ILE:HD13	2.01	0.42
1:G:61:ASP:OD1	1:G:241:ASN:ND2	2.43	0.42
1:A:260:ILE:HD11	1:B:280:ALA:CB	2.50	0.41
1:B:79:THR:O	1:B:462:PHE:HA	2.20	0.41
1:E:517:ILE:HD13	1:E:520:LEU:HD12	2.02	0.41
1:A:108:THR:HA	1:C:85:PRO:HG2	2.02	0.41
1:B:483:SER:HA	1:D:78:PHE:HE2	1.85	0.41
1:E:360:LYS:HD2	1:E:360:LYS:N	2.35	0.41
1:E:525:SER:CB	1:E:529:THR:HG23	2.47	0.41
1:F:219:VAL:HG13	1:F:220:PRO:HD2	1.95	0.41
1:F:251:GLU:HB2	1:F:401:MET:HE2	2.01	0.41
1:G:232:ARG:HD3	1:G:232:ARG:C	2.42	0.41
1:G:259:THR:HG22	1:G:268:ILE:HD13	2.01	0.41
1:B:145:GLN:NE2	1:B:163:ILE:O	2.49	0.41
1:B:288:SER:C	1:B:289:LYS:HD3	2.46	0.41
1:E:483:SER:HA	1:G:78:PHE:HE2	1.84	0.41
1:F:108:THR:O	1:H:133:HIS:NE2	2.52	0.41
1:F:251:GLU:CB	1:F:401:MET:HE2	2.51	0.41
1:F:504:GLU:H	1:F:504:GLU:HG2	1.50	0.41
1:G:385:ALA:HB2	1:G:401:MET:HE3	1.94	0.41
1:G:517:ILE:HD13	1:G:520:LEU:HD12	2.02	0.41
1:A:1:MET:H3	1:A:2:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:GLU:O	1:C:507:LYS:HG3	2.20	0.41
1:D:285:GLU:O	1:D:289:LYS:HG3	2.20	0.41
1:E:498:GLU:CG	1:E:503:VAL:HG11	2.49	0.41
1:H:160:THR:HA	1:H:161:PRO:HD3	1.87	0.41
1:C:199:HIS:HB3	1:C:245:VAL:HB	2.01	0.41
1:C:201:GLU:C	1:C:224:HIS:CE1	2.98	0.41
1:A:79:THR:O	1:A:462:PHE:HA	2.20	0.41
1:B:259:THR:HG22	1:B:268:ILE:HD13	2.01	0.41
1:C:79:THR:O	1:C:462:PHE:HA	2.20	0.41
1:C:177:HIS:CD2	4:C:712:HOH:O	2.58	0.41
1:F:111:THR:N	1:F:126:THR:HG22	2.33	0.41
1:G:127:VAL:N	1:G:128:PRO:CD	2.83	0.41
1:H:259:THR:HG22	1:H:268:ILE:HD13	2.01	0.41
1:A:291:ILE:HD12	1:A:291:ILE:N	2.35	0.41
1:B:393:ALA:HB3	1:B:394:PRO:HD3	2.03	0.41
1:C:51:LYS:NZ	4:C:705:HOH:O	2.53	0.41
1:C:124:MET:HE1	1:D:121:ASP:O	2.21	0.41
1:D:211:GLY:HA3	1:D:402:GLU:OE1	2.21	0.41
1:E:324:ASN:HD22	1:E:324:ASN:H	1.67	0.41
1:A:441:MET:HE1	1:A:446:GLN:HA	2.02	0.41
1:B:86:ILE:HD11	1:D:468:LEU:HD12	2.03	0.41
1:E:66:LEU:O	1:E:70:HIS:HD2	2.04	0.41
1:E:211:GLY:HA3	1:E:402:GLU:OE1	2.21	0.41
1:G:84:ASP:OD1	1:G:84:ASP:C	2.64	0.41
1:H:366:TRP:CD1	1:H:366:TRP:C	2.98	0.41
1:A:84:ASP:HB2	1:A:85:PRO:CD	2.51	0.41
1:A:211:GLY:HA3	1:A:402:GLU:OE1	2.21	0.41
1:A:539:THR:CG2	1:C:212:HIS:HB3	2.51	0.41
1:B:211:GLY:HA3	1:B:402:GLU:OE1	2.21	0.41
1:B:517:ILE:HD13	1:B:520:LEU:HD12	2.03	0.41
1:C:61:ASP:OD1	1:C:241:ASN:ND2	2.43	0.41
1:C:382:THR:O	1:C:386:VAL:HG23	2.21	0.41
1:C:393:ALA:HB3	1:C:394:PRO:HD3	2.03	0.41
1:C:517:ILE:HD13	1:C:520:LEU:HD12	2.02	0.41
1:E:84:ASP:HB2	1:E:85:PRO:CD	2.51	0.41
1:E:189:MET:O	1:E:193:ARG:CG	2.67	0.41
1:F:328:LYS:HB2	4:F:707:HOH:O	2.20	0.41
1:F:408:TYR:HE2	1:F:452:ARG:HB3	1.86	0.41
1:G:251:GLU:CB	1:G:401:MET:HE2	2.51	0.41
1:H:79:THR:O	1:H:462:PHE:HA	2.21	0.41
1:H:127:VAL:N	1:H:128:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:208:LYS:O	1:H:208:LYS:HG3	2.20	0.41
1:H:517:ILE:HD13	1:H:520:LEU:HD12	2.03	0.41
1:B:483:SER:HA	1:D:78:PHE:CE2	2.56	0.41
1:F:448:THR:HG23	1:F:452:ARG:HD3	2.03	0.41
1:E:342:LEU:HD12	1:E:342:LEU:H	1.86	0.40
1:F:127:VAL:N	1:F:128:PRO:CD	2.83	0.40
1:F:366:TRP:CD1	1:F:366:TRP:C	2.99	0.40
1:F:393:ALA:HB3	1:F:394:PRO:HD3	2.03	0.40
1:F:429:TYR:CD2	1:F:431:LEU:HD22	2.54	0.40
1:A:259:THR:HG22	1:A:268:ILE:HD13	2.02	0.40
1:A:382:THR:O	1:A:386:VAL:HG23	2.21	0.40
1:A:393:ALA:N	1:A:394:PRO:HD2	2.36	0.40
1:A:485:ILE:CG2	1:A:489:ALA:HB2	2.51	0.40
1:C:92:ALA:HB1	1:C:164:ASP:O	2.21	0.40
1:C:259:THR:HG22	1:C:268:ILE:HD13	2.02	0.40
1:C:491:GLY:O	1:C:496:GLN:HB2	2.21	0.40
1:C:518:ASP:OD1	1:C:518:ASP:C	2.63	0.40
1:D:317:ILE:HG23	1:D:318:ASP:N	2.36	0.40
1:F:8:ILE:HD11	1:G:158:ALA:HA	2.03	0.40
1:F:79:THR:O	1:F:462:PHE:HA	2.21	0.40
1:F:393:ALA:N	1:F:394:PRO:HD2	2.36	0.40
1:G:382:THR:O	1:G:386:VAL:HG23	2.22	0.40
1:H:63:LEU:HD12	1:H:243:LEU:CD2	2.51	0.40
1:A:92:ALA:HB1	1:A:164:ASP:O	2.22	0.40
1:A:127:VAL:N	1:A:128:PRO:CD	2.84	0.40
1:A:167:ARG:HA	1:A:168:PRO:HD3	1.96	0.40
1:A:285:GLU:O	1:A:289:LYS:HG3	2.20	0.40
1:A:441:MET:CE	1:A:446:GLN:HA	2.51	0.40
1:B:382:THR:O	1:B:386:VAL:HG23	2.21	0.40
1:C:393:ALA:N	1:C:394:PRO:HD2	2.36	0.40
1:D:382:THR:O	1:D:386:VAL:HG23	2.21	0.40
1:E:92:ALA:HB1	1:E:164:ASP:O	2.21	0.40
1:E:382:THR:O	1:E:386:VAL:HG23	2.20	0.40
1:G:92:ALA:HB1	1:G:164:ASP:O	2.21	0.40
1:H:84:ASP:HB2	1:H:85:PRO:CD	2.51	0.40
1:H:393:ALA:HB3	1:H:394:PRO:HD3	2.03	0.40
1:A:6:ILE:HD11	1:D:149:ARG:NH2	2.36	0.40
1:D:259:THR:HG22	1:D:268:ILE:HD13	2.02	0.40
1:F:92:ALA:HB1	1:F:164:ASP:O	2.22	0.40
1:F:211:GLY:HA3	1:F:402:GLU:OE1	2.21	0.40
1:G:84:ASP:HB2	1:G:85:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:393:ALA:HB3	1:G:394:PRO:HD3	2.03	0.40
1:B:84:ASP:OD1	1:B:84:ASP:C	2.64	0.40
1:E:85:PRO:HG2	1:G:108:THR:HA	2.04	0.40
1:H:167:ARG:HA	1:H:168:PRO:HD3	1.95	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLU:OE1	1:H:321:LYS:NZ[1_565]	1.54	0.66
1:D:324:ASN:N	1:H:322:ASN:O[2_555]	2.04	0.16
1:B:289:LYS:CG	1:F:282:LEU:CD1[2_456]	2.10	0.10

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	542/556 (98%)	532 (98%)	10 (2%)	0	100	100
1	B	538/556 (97%)	528 (98%)	10 (2%)	0	100	100
1	C	531/556 (96%)	520 (98%)	11 (2%)	0	100	100
1	D	537/556 (97%)	527 (98%)	10 (2%)	0	100	100
1	E	538/556 (97%)	526 (98%)	12 (2%)	0	100	100
1	F	541/556 (97%)	531 (98%)	10 (2%)	0	100	100
1	G	531/556 (96%)	521 (98%)	10 (2%)	0	100	100
1	H	529/556 (95%)	516 (98%)	13 (2%)	0	100	100
All	All	4287/4448 (96%)	4201 (98%)	86 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/456 (98%)	423 (95%)	23 (5%)	21	47
1	B	442/456 (97%)	414 (94%)	28 (6%)	16	39
1	C	439/456 (96%)	421 (96%)	18 (4%)	27	56
1	D	444/456 (97%)	414 (93%)	30 (7%)	14	35
1	E	445/456 (98%)	413 (93%)	32 (7%)	13	32
1	F	445/456 (98%)	415 (93%)	30 (7%)	15	36
1	G	438/456 (96%)	411 (94%)	27 (6%)	16	39
1	H	434/456 (95%)	408 (94%)	26 (6%)	17	41
All	All	3533/3648 (97%)	3319 (94%)	214 (6%)	17	40

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	9	GLN
1	A	33	LYS
1	A	51	LYS
1	A	66	LEU
1	A	74	LYS
1	A	75	THR
1	A	116	SER
1	A	155	GLU
1	A	201	GLU
1	A	208	LYS
1	A	262	HIS
1	A	269	ILE
1	A	296	LEU
1	A	306	LYS
1	A	327	ASN
1	A	345	THR
1	A	398	LEU
1	A	439	LYS

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Mol	Chain	Res	Type
1	A	444	ASP
1	A	494	VAL
1	A	496	GLN
1	A	528	VAL
1	B	6	ILE
1	B	24	LYS
1	B	30	ARG
1	B	32	ARG
1	B	41	GLU
1	B	51	LYS
1	B	66	LEU
1	B	69	LYS
1	B	74	LYS
1	B	75	THR
1	B	116	SER
1	B	148	GLU
1	B	157	ARG
1	B	193	ARG
1	B	201	GLU
1	B	208	LYS
1	B	269	ILE
1	B	283	MET
1	B	296	LEU
1	B	302	GLU
1	B	331	LEU
1	B	332	ILE
1	B	345	THR
1	B	398	LEU
1	B	439	LYS
1	B	496	GLN
1	B	509	GLN
1	B	528	VAL
1	C	6	ILE
1	C	33	LYS
1	C	51	LYS
1	C	66	LEU
1	C	116	SER
1	C	145	GLN
1	C	155	GLU
1	C	201	GLU
1	C	208	LYS
1	C	269	ILE

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Mol	Chain	Res	Type
1	C	287	GLU
1	C	324	ASN
1	C	345	THR
1	C	398	LEU
1	C	439	LYS
1	C	494	VAL
1	C	496	GLN
1	C	528	VAL
1	D	6	ILE
1	D	24	LYS
1	D	32	ARG
1	D	33	LYS
1	D	51	LYS
1	D	65	LYS
1	D	66	LEU
1	D	75	THR
1	D	116	SER
1	D	155	GLU
1	D	201	GLU
1	D	208	LYS
1	D	269	ILE
1	D	294	ASN
1	D	296	LEU
1	D	302	GLU
1	D	305	LYS
1	D	317	ILE
1	D	327	ASN
1	D	336	THR
1	D	345	THR
1	D	348	LYS
1	D	368	VAL
1	D	382	THR
1	D	398	LEU
1	D	439	LYS
1	D	494	VAL
1	D	496	GLN
1	D	505	VAL
1	D	528	VAL
1	E	6	ILE
1	E	51	LYS
1	E	66	LEU
1	E	108	THR

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Mol	Chain	Res	Type
1	E	113	ASN
1	E	116	SER
1	E	145	GLN
1	E	175	THR
1	E	193	ARG
1	E	201	GLU
1	E	208	LYS
1	E	243	LEU
1	E	263	ARG
1	E	269	ILE
1	E	283	MET
1	E	289	LYS
1	E	291	ILE
1	E	296	LEU
1	E	322	ASN
1	E	324	ASN
1	E	332	ILE
1	E	334	LYS
1	E	336	THR
1	E	345	THR
1	E	368	VAL
1	E	382	THR
1	E	398	LEU
1	E	439	LYS
1	E	444	ASP
1	E	494	VAL
1	E	504	GLU
1	E	528	VAL
1	F	6	ILE
1	F	33	LYS
1	F	51	LYS
1	F	61	ASP
1	F	66	LEU
1	F	75	THR
1	F	116	SER
1	F	126	THR
1	F	155	GLU
1	F	187	THR
1	F	201	GLU
1	F	208	LYS
1	F	225	ILE
1	F	237	ILE

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Mol	Chain	Res	Type
1	F	269	ILE
1	F	296	LEU
1	F	321	LYS
1	F	322	ASN
1	F	331	LEU
1	F	345	THR
1	F	368	VAL
1	F	386	VAL
1	F	398	LEU
1	F	431	LEU
1	F	439	LYS
1	F	496	GLN
1	F	504	GLU
1	F	528	VAL
1	F	531	THR
1	F	541	ASP
1	G	6	ILE
1	G	19	VAL
1	G	32	ARG
1	G	33	LYS
1	G	51	LYS
1	G	66	LEU
1	G	113	ASN
1	G	116	SER
1	G	152	LEU
1	G	201	GLU
1	G	232	ARG
1	G	269	ILE
1	G	289	LYS
1	G	296	LEU
1	G	299	ILE
1	G	302	GLU
1	G	305	LYS
1	G	322	ASN
1	G	345	THR
1	G	355	LYS
1	G	360	LYS
1	G	398	LEU
1	G	439	LYS
1	G	444	ASP
1	G	494	VAL
1	G	496	GLN

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Mol	Chain	Res	Type
1	G	528	VAL
1	H	4	THR
1	H	6	ILE
1	H	33	LYS
1	H	37	ILE
1	H	51	LYS
1	H	63	LEU
1	H	66	LEU
1	H	75	THR
1	H	113	ASN
1	H	116	SER
1	H	155	GLU
1	H	201	GLU
1	H	208	LYS
1	H	269	ILE
1	H	292	TYR
1	H	296	LEU
1	H	336	THR
1	H	342	LEU
1	H	345	THR
1	H	348	LYS
1	H	398	LEU
1	H	439	LYS
1	H	444	ASP
1	H	473	LEU
1	H	496	GLN
1	H	528	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	70	HIS
1	A	327	ASN
1	A	469	HIS
1	A	492	GLN
1	B	133	HIS
1	B	212	HIS
1	B	262	HIS
1	B	425	GLN
1	B	509	GLN
1	C	54	HIS

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Mol	Chain	Res	Type
1	C	58	GLN
1	C	87	HIS
1	C	177	HIS
1	C	212	HIS
1	C	262	HIS
1	C	495	GLN
1	C	508	HIS
1	C	536	GLN
1	D	212	HIS
1	D	327	ASN
1	E	53	ASN
1	E	54	HIS
1	E	113	ASN
1	E	138	GLN
1	E	212	HIS
1	E	324	ASN
1	E	425	GLN
1	E	492	GLN
1	E	508	HIS
1	E	542	GLN
1	F	53	ASN
1	F	54	HIS
1	F	70	HIS
1	F	133	HIS
1	F	138	GLN
1	F	203	GLN
1	F	212	HIS
1	F	222	GLN
1	F	436	ASN
1	F	492	GLN
1	F	508	HIS
1	G	104	GLN
1	G	113	ASN
1	G	212	HIS
1	G	492	GLN
1	G	508	HIS
1	H	104	GLN
1	H	113	ASN
1	H	212	HIS
1	H	383	GLN
1	H	410	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\# Z > 2$
3	FMT	B	602	-	2,2,2	0.71	0	1,1,1	0.68	0
3	FMT	G	602	-	2,2,2	0.69	0	1,1,1	0.69	0
3	FMT	G	603	-	2,2,2	0.65	0	1,1,1	0.71	0
3	FMT	D	603	-	2,2,2	0.67	0	1,1,1	0.70	0
3	FMT	H	602	-	2,2,2	0.70	0	1,1,1	0.69	0
3	FMT	H	603	-	2,2,2	0.68	0	1,1,1	0.69	0
3	FMT	B	603	-	2,2,2	0.68	0	1,1,1	0.70	0
3	FMT	C	603	-	2,2,2	0.65	0	1,1,1	0.71	0
3	FMT	D	602	2	2,2,2	0.67	0	1,1,1	0.70	0
3	FMT	A	603	-	2,2,2	0.67	0	1,1,1	0.70	0
3	FMT	A	602	-	2,2,2	0.67	0	1,1,1	0.72	0
3	FMT	C	602	-	2,2,2	0.65	0	1,1,1	0.73	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.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	603	FMT	1	0
3	D	603	FMT	1	0
3	H	603	FMT	2	0
3	B	603	FMT	2	0

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	544/556 (97%)	-0.12	1 (0%) 91 90	43, 66, 103, 132	0
1	B	540/556 (97%)	-0.09	2 (0%) 88 87	42, 67, 101, 121	0
1	C	535/556 (96%)	-0.10	4 (0%) 84 83	39, 66, 111, 127	0
1	D	541/556 (97%)	-0.12	2 (0%) 88 87	39, 63, 98, 123	0
1	E	542/556 (97%)	0.09	3 (0%) 85 85	54, 82, 116, 136	0
1	F	543/556 (97%)	0.21	2 (0%) 88 87	50, 80, 113, 132	0
1	G	535/556 (96%)	0.00	4 (0%) 84 83	40, 74, 117, 138	0
1	H	533/556 (95%)	0.00	4 (0%) 82 81	48, 71, 113, 140	0
All	All	4313/4448 (96%)	-0.02	22 (0%) 87 86	39, 71, 111, 140	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	PRO	3.4
1	G	296	LEU	3.1
1	A	210	CYS	3.0
1	F	215	GLY	2.8
1	H	532	ALA	2.8
1	G	299	ILE	2.7
1	F	2	PRO	2.6
1	B	2	PRO	2.6
1	H	528	VAL	2.5
1	G	515	THR	2.4
1	E	450	ILE	2.4
1	B	270	GLY	2.4
1	D	526	GLY	2.4
1	E	210	CYS	2.3
1	C	297	ALA	2.2
1	C	299	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	291	ILE	2.2
1	H	521	LEU	2.2
1	G	290	GLY	2.1
1	C	533	ALA	2.1
1	E	529	THR	2.1
1	H	292	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FMT	B	602	3/3	0.87	0.16	78,78,83,84	0
3	FMT	H	602	3/3	0.87	0.15	68,68,71,76	0
3	FMT	B	603	3/3	0.89	0.15	75,75,80,81	0
2	MG	B	601	1/1	0.89	0.11	63,63,63,63	0
3	FMT	D	602	3/3	0.90	0.13	63,63,63,72	0
3	FMT	D	603	3/3	0.91	0.22	75,75,83,83	0
3	FMT	G	602	3/3	0.91	0.10	69,69,76,80	0
2	MG	G	601	1/1	0.91	0.12	62,62,62,62	0
3	FMT	H	603	3/3	0.92	0.16	76,76,81,84	0
3	FMT	C	603	3/3	0.93	0.10	63,63,67,72	0
2	MG	F	601	1/1	0.93	0.15	71,71,71,71	0
2	MG	E	601	1/1	0.93	0.14	69,69,69,69	0
3	FMT	C	602	3/3	0.94	0.09	68,68,69,73	0
3	FMT	A	603	3/3	0.95	0.21	76,76,82,84	0
3	FMT	A	602	3/3	0.95	0.12	70,70,72,76	0
2	MG	H	601	1/1	0.96	0.05	70,70,70,70	0
2	MG	D	601	1/1	0.97	0.06	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FMT	G	603	3/3	0.97	0.06	74,74,74,75	0
2	MG	C	601	1/1	0.98	0.06	52,52,52,52	0
2	MG	A	601	1/1	0.98	0.05	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.