



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:32 AM UTC

PDB ID : 4E2L / pdb_00004e2l
Title : Crystal Structure of the periplasmic domain of mutant FepE LPS O-antigen chain length regulator protein
Authors : Kalynych, S.; Yao, D.; Magee, J.D.; Cygler, M.
Deposited on : 2012-03-08
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

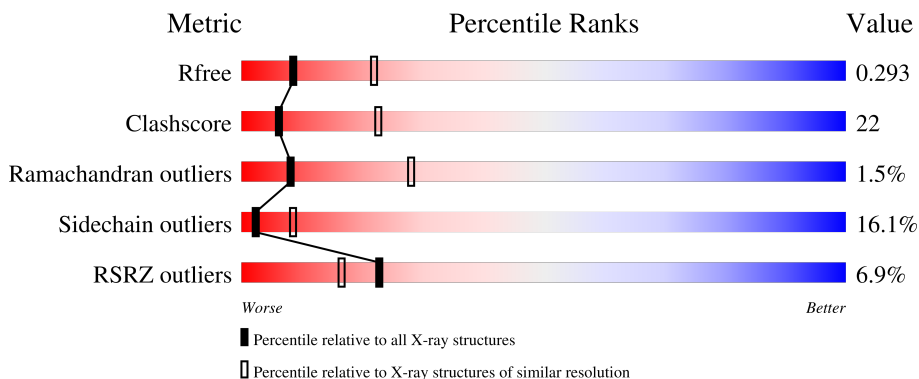
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.





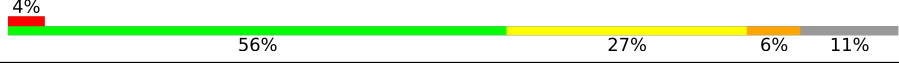
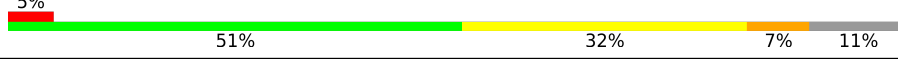
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	271	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 46%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6% 46% 30% 12% 11%</p>
1	B	271	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 52%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6% 52% 29% 7% 11%</p>
1	C	271	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">10% 48% 32% 10% 9%</p>
1	D	271	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 52%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7% 52% 30% 6% 11%</p>
1	E	271	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 52%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6% 52% 30% 6% 11%</p>

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Mol	Chain	Length	Quality of chain
1	F	271	
1	G	271	
1	H	271	
1	I	271	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 16883 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 Ferric enterobactin (Enterochelin) transport.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	240	Total 1881	C 1204	N 306	O 368	S 3	0	0	0
1	B	240	Total 1903	C 1213	N 317	O 370	S 3	0	0	0
1	C	246	Total 1893	C 1209	N 314	O 367	S 3	0	0	0
1	D	240	Total 1869	C 1195	N 309	O 362	S 3	0	0	0
1	E	241	Total 1848	C 1178	N 301	O 366	S 3	0	0	0
1	F	244	Total 1898	C 1214	N 314	O 367	S 3	0	0	0
1	G	240	Total 1859	C 1193	N 303	O 360	S 3	0	0	0
1	H	242	Total 1858	C 1190	N 306	O 359	S 3	0	0	0
1	I	242	Total 1874	C 1198	N 314	O 359	S 3	0	0	0

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	HIS	-	expression tag	UNP Q8XBV8
A	58	HIS	-	expression tag	UNP Q8XBV8
A	59	HIS	-	expression tag	UNP Q8XBV8
A	60	HIS	-	expression tag	UNP Q8XBV8
A	61	HIS	-	expression tag	UNP Q8XBV8
A	62	HIS	-	expression tag	UNP Q8XBV8
A	63	GLY	-	expression tag	UNP Q8XBV8
A	64	SER	-	expression tag	UNP Q8XBV8
A	262	GLY	-	linker	UNP Q8XBV8
A	263	SER	-	linker	UNP Q8XBV8
A	264	GLY	-	linker	UNP Q8XBV8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	57	HIS	-	expression tag	UNP Q8XBV8
B	58	HIS	-	expression tag	UNP Q8XBV8
B	59	HIS	-	expression tag	UNP Q8XBV8
B	60	HIS	-	expression tag	UNP Q8XBV8
B	61	HIS	-	expression tag	UNP Q8XBV8
B	62	HIS	-	expression tag	UNP Q8XBV8
B	63	GLY	-	expression tag	UNP Q8XBV8
B	64	SER	-	expression tag	UNP Q8XBV8
B	262	GLY	-	linker	UNP Q8XBV8
B	263	SER	-	linker	UNP Q8XBV8
B	264	GLY	-	linker	UNP Q8XBV8
C	57	HIS	-	expression tag	UNP Q8XBV8
C	58	HIS	-	expression tag	UNP Q8XBV8
C	59	HIS	-	expression tag	UNP Q8XBV8
C	60	HIS	-	expression tag	UNP Q8XBV8
C	61	HIS	-	expression tag	UNP Q8XBV8
C	62	HIS	-	expression tag	UNP Q8XBV8
C	63	GLY	-	expression tag	UNP Q8XBV8
C	64	SER	-	expression tag	UNP Q8XBV8
C	262	GLY	-	linker	UNP Q8XBV8
C	263	SER	-	linker	UNP Q8XBV8
C	264	GLY	-	linker	UNP Q8XBV8
D	57	HIS	-	expression tag	UNP Q8XBV8
D	58	HIS	-	expression tag	UNP Q8XBV8
D	59	HIS	-	expression tag	UNP Q8XBV8
D	60	HIS	-	expression tag	UNP Q8XBV8
D	61	HIS	-	expression tag	UNP Q8XBV8
D	62	HIS	-	expression tag	UNP Q8XBV8
D	63	GLY	-	expression tag	UNP Q8XBV8
D	64	SER	-	expression tag	UNP Q8XBV8
D	262	GLY	-	linker	UNP Q8XBV8
D	263	SER	-	linker	UNP Q8XBV8
D	264	GLY	-	linker	UNP Q8XBV8
E	57	HIS	-	expression tag	UNP Q8XBV8
E	58	HIS	-	expression tag	UNP Q8XBV8
E	59	HIS	-	expression tag	UNP Q8XBV8
E	60	HIS	-	expression tag	UNP Q8XBV8
E	61	HIS	-	expression tag	UNP Q8XBV8
E	62	HIS	-	expression tag	UNP Q8XBV8
E	63	GLY	-	expression tag	UNP Q8XBV8
E	64	SER	-	expression tag	UNP Q8XBV8
E	262	GLY	-	linker	UNP Q8XBV8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	263	SER	-	linker	UNP Q8XBV8
E	264	GLY	-	linker	UNP Q8XBV8
F	57	HIS	-	expression tag	UNP Q8XBV8
F	58	HIS	-	expression tag	UNP Q8XBV8
F	59	HIS	-	expression tag	UNP Q8XBV8
F	60	HIS	-	expression tag	UNP Q8XBV8
F	61	HIS	-	expression tag	UNP Q8XBV8
F	62	HIS	-	expression tag	UNP Q8XBV8
F	63	GLY	-	expression tag	UNP Q8XBV8
F	64	SER	-	expression tag	UNP Q8XBV8
F	262	GLY	-	linker	UNP Q8XBV8
F	263	SER	-	linker	UNP Q8XBV8
F	264	GLY	-	linker	UNP Q8XBV8
G	57	HIS	-	expression tag	UNP Q8XBV8
G	58	HIS	-	expression tag	UNP Q8XBV8
G	59	HIS	-	expression tag	UNP Q8XBV8
G	60	HIS	-	expression tag	UNP Q8XBV8
G	61	HIS	-	expression tag	UNP Q8XBV8
G	62	HIS	-	expression tag	UNP Q8XBV8
G	63	GLY	-	expression tag	UNP Q8XBV8
G	64	SER	-	expression tag	UNP Q8XBV8
G	262	GLY	-	linker	UNP Q8XBV8
G	263	SER	-	linker	UNP Q8XBV8
G	264	GLY	-	linker	UNP Q8XBV8
H	57	HIS	-	expression tag	UNP Q8XBV8
H	58	HIS	-	expression tag	UNP Q8XBV8
H	59	HIS	-	expression tag	UNP Q8XBV8
H	60	HIS	-	expression tag	UNP Q8XBV8
H	61	HIS	-	expression tag	UNP Q8XBV8
H	62	HIS	-	expression tag	UNP Q8XBV8
H	63	GLY	-	expression tag	UNP Q8XBV8
H	64	SER	-	expression tag	UNP Q8XBV8
H	262	GLY	-	linker	UNP Q8XBV8
H	263	SER	-	linker	UNP Q8XBV8
H	264	GLY	-	linker	UNP Q8XBV8
I	57	HIS	-	expression tag	UNP Q8XBV8
I	58	HIS	-	expression tag	UNP Q8XBV8
I	59	HIS	-	expression tag	UNP Q8XBV8
I	60	HIS	-	expression tag	UNP Q8XBV8
I	61	HIS	-	expression tag	UNP Q8XBV8
I	62	HIS	-	expression tag	UNP Q8XBV8
I	63	GLY	-	expression tag	UNP Q8XBV8

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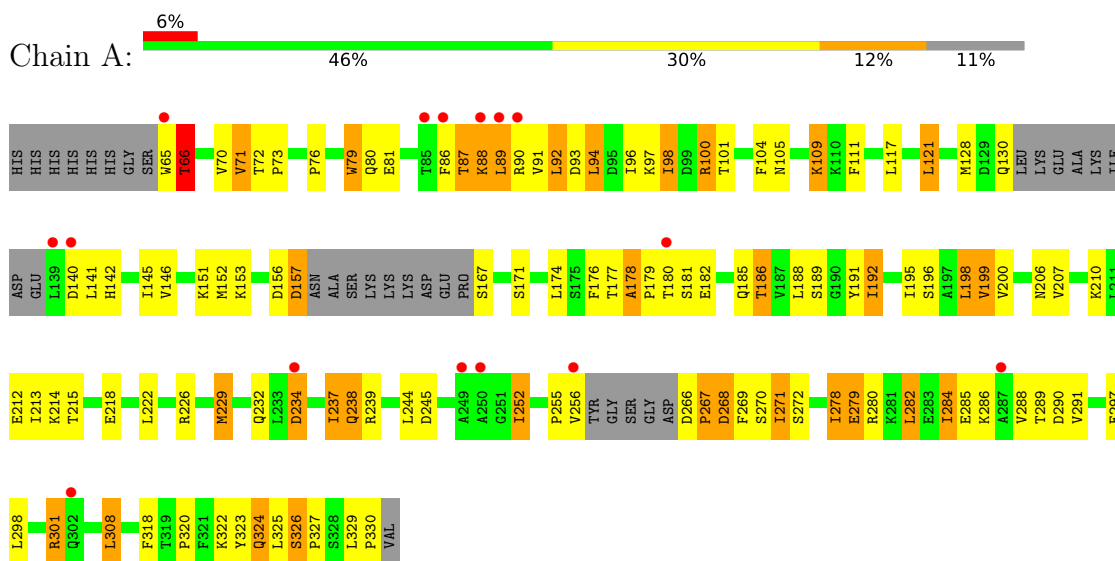
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Chain	Residue	Modelled	Actual	Comment	Reference
I	64	SER	-	expression tag	UNP Q8XBV8
I	262	GLY	-	linker	UNP Q8XBV8
I	263	SER	-	linker	UNP Q8XBV8
I	264	GLY	-	linker	UNP Q8XBV8

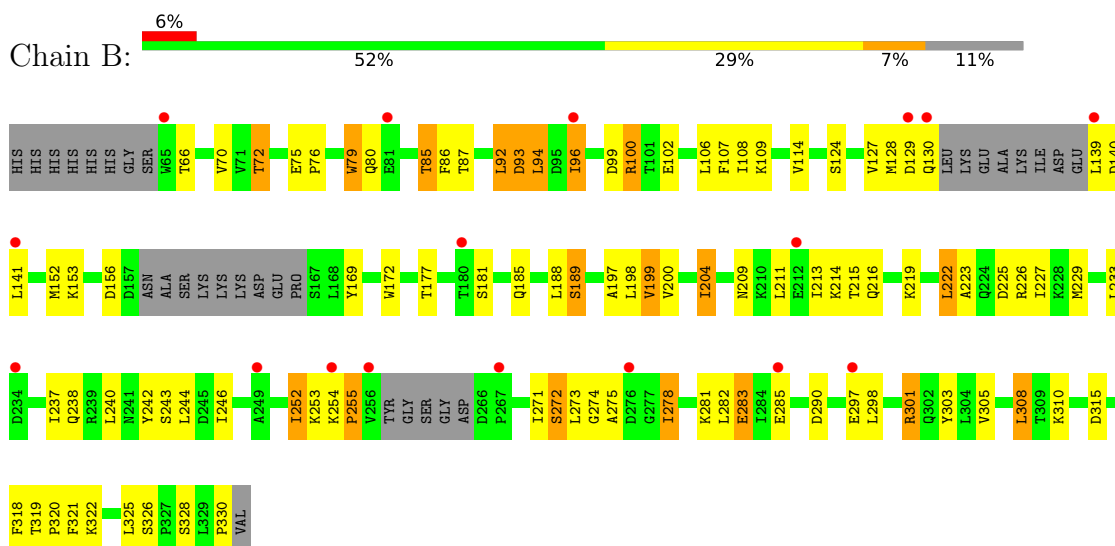
3 Residue-property plots [i](#)

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: Ferric enterobactin (Enterochelin) transport

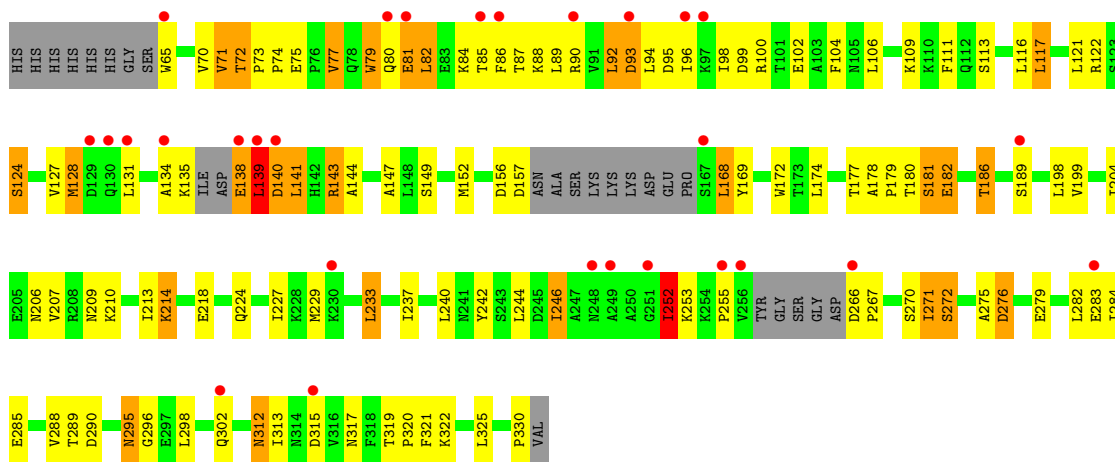


- Molecule 1: Ferric enterobactin (Enterochelin) transport

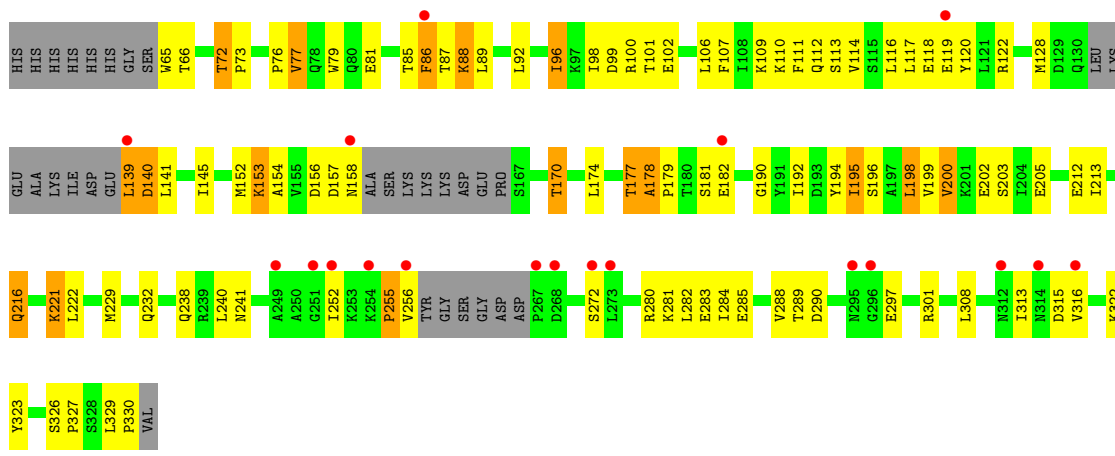


- Molecule 1: Ferric enterobactin (Enterochelin) transport

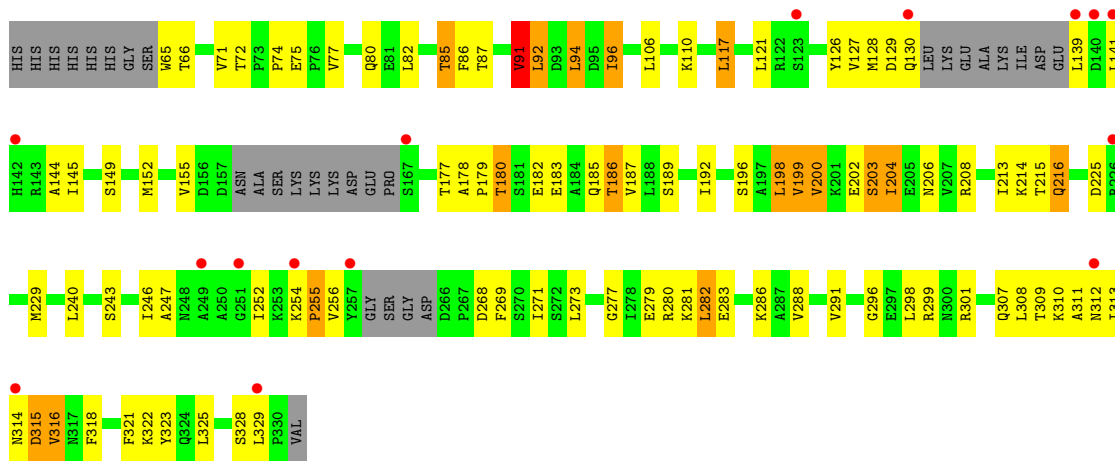


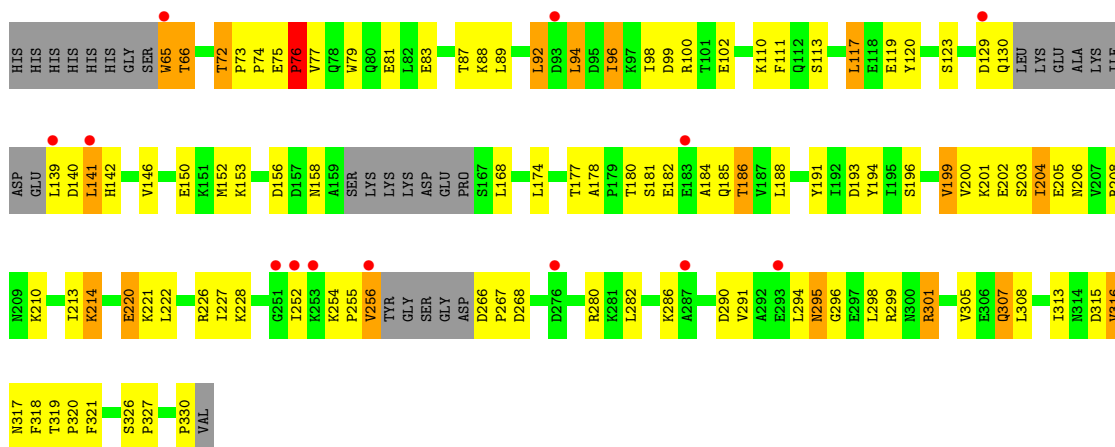


• Molecule 1: Ferric enterobactin (Enterochelin) transport



• Molecule 1: Ferric enterobactin (Enterochelin) transport





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.31Å 141.26Å 136.89Å 90.00° 107.03° 90.00°	Depositor
Resolution (Å)	49.72 – 2.80 49.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.8 (49.72-2.80) 99.0 (49.72-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	11.30	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.15 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.242 , 0.289 0.245 , 0.293	Depositor DCC
R_{free} test set	4693 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtrriage
Anisotropy	0.341	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16883	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.88% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.63	0/1911	0.97	6/2594 (0.2%)
1	B	0.55	0/1932	0.86	0/2617
1	C	0.56	0/1923	0.93	5/2617 (0.2%)
1	D	0.57	0/1899	0.88	3/2577 (0.1%)
1	E	0.61	0/1877	0.95	2/2557 (0.1%)
1	F	0.58	0/1928	0.92	5/2618 (0.2%)
1	G	0.60	0/1889	0.88	4/2566 (0.2%)
1	H	0.57	0/1887	0.89	2/2565 (0.1%)
1	I	0.57	0/1903	0.92	5/2585 (0.2%)
All	All	0.58	0/17149	0.91	32/23296 (0.1%)

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	1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ALA	N-CA-C	8.01	115.43	108.22
1	H	140	ASP	N-CA-C	-6.93	104.57	113.16
1	F	324	GLN	N-CA-C	-6.83	105.07	113.41
1	A	66	THR	N-CA-C	6.62	119.20	108.34
1	I	254	LYS	CA-C-N	6.60	128.09	119.84
1	I	254	LYS	C-N-CA	6.60	128.09	119.84
1	G	266	ASP	CA-C-N	6.46	125.68	118.97
1	G	266	ASP	C-N-CA	6.46	125.68	118.97
1	I	75	GLU	CA-C-N	6.36	127.79	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	75	GLU	C-N-CA	6.36	127.79	119.84
1	A	140	ASP	N-CA-C	-6.20	105.69	113.20
1	C	295	ASN	N-CA-C	6.02	119.05	109.24
1	A	324	GLN	N-CA-C	-5.90	104.20	111.40
1	C	178	ALA	CA-C-N	5.88	127.19	119.84
1	C	178	ALA	C-N-CA	5.88	127.19	119.84
1	F	128	MET	N-CA-C	5.78	118.36	111.71
1	C	275	ALA	N-CA-C	5.59	118.09	111.33
1	H	128	MET	N-CA-C	5.55	119.23	112.23
1	F	178	ALA	CA-C-N	5.52	126.74	119.84
1	F	178	ALA	C-N-CA	5.52	126.74	119.84
1	D	178	ALA	N-CA-C	5.30	112.79	108.07
1	G	178	ALA	CA-C-N	5.20	126.33	119.84
1	G	178	ALA	C-N-CA	5.20	126.33	119.84
1	D	178	ALA	CA-C-N	5.19	124.64	119.24
1	D	178	ALA	C-N-CA	5.19	124.64	119.24
1	E	254	LYS	CA-C-N	5.19	126.32	119.84
1	E	254	LYS	C-N-CA	5.19	126.32	119.84
1	F	295	ASN	N-CA-C	5.13	117.26	108.90
1	A	297	GLU	CA-C-N	5.10	127.83	120.38
1	A	297	GLU	C-N-CA	5.10	127.83	120.38
1	C	124	SER	N-CA-C	5.08	116.93	109.42
1	I	295	ASN	N-CA-C	5.03	117.53	107.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	THR	Peptide

5.2 Too-close contacts [i](#)

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	1881	0	1854	118	0
1	B	1903	0	1909	90	0
1	C	1893	0	1832	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1869	0	1830	81	0
1	E	1848	0	1780	87	0
1	F	1898	0	1862	108	0
1	G	1859	0	1827	81	0
1	H	1858	0	1823	71	0
1	I	1874	0	1856	84	0
All	All	16883	0	16573	748	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 22.

All (748) 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:G:79:TRP:CZ2	1:G:98:ILE:HD11	1.80	1.16
1:A:222:LEU:HD13	1:A:301:ARG:HG2	1.27	1.15
1:I:301:ARG:HG2	1:I:301:ARG:HH21	1.06	1.11
1:G:280:ARG:HG3	1:G:280:ARG:HH11	1.08	1.11
1:B:301:ARG:HH11	1:B:301:ARG:HG2	1.10	1.08
1:G:79:TRP:HZ2	1:G:98:ILE:HD11	1.10	1.06
1:A:94:LEU:HG	1:A:214:LYS:HD2	1.31	1.06
1:F:94:LEU:HG	1:F:214:LYS:HG3	1.37	1.06
1:A:284:ILE:HG12	1:B:242:TYR:HD1	1.16	1.04
1:G:106:LEU:HD23	1:G:199:VAL:HG23	1.43	1.00
1:H:301:ARG:HG2	1:H:301:ARG:HH11	1.21	1.00
1:B:255:PRO:HG2	1:C:252:ILE:HD11	1.44	0.98
1:D:153:LYS:HD2	1:D:154:ALA:H	1.26	0.95
1:E:66:THR:HG22	1:E:177:THR:OG1	1.66	0.94
1:G:94:LEU:HD22	1:G:96:ILE:HG12	1.46	0.94
1:E:255:PRO:HG2	1:F:252:ILE:HD11	1.49	0.94
1:A:284:ILE:HG12	1:B:242:TYR:CD1	2.03	0.93
1:C:86:PHE:HZ	1:C:98:ILE:HG13	1.33	0.93
1:F:255:PRO:HG2	1:G:252:ILE:HD11	1.48	0.92
1:G:66:THR:OG1	1:G:177:THR:HB	1.71	0.89
1:E:208:ARG:HG2	1:E:313:ILE:CG2	2.03	0.88
1:I:301:ARG:HG2	1:I:301:ARG:NH2	1.87	0.87
1:B:301:ARG:HG2	1:B:301:ARG:NH1	1.90	0.86
1:H:301:ARG:HG2	1:H:301:ARG:NH1	1.87	0.86
1:G:280:ARG:HH11	1:G:280:ARG:CG	1.87	0.86
1:D:86:PHE:CD1	1:D:96:ILE:HG22	2.11	0.86
1:F:180:THR:HG23	1:F:183:GLU:HB3	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:LEU:H	1:I:141:LEU:HD23	1.41	0.86
1:C:72:THR:HG22	1:C:322:LYS:HB3	1.55	0.85
1:F:208:ARG:O	1:F:212:GLU:HG2	1.77	0.84
1:H:301:ARG:HH11	1:H:301:ARG:CG	1.90	0.84
1:D:222:LEU:HD13	1:D:301:ARG:HB3	1.60	0.84
1:E:85:THR:CG2	1:E:313:ILE:HD11	2.07	0.83
1:F:65:TRP:HE3	1:F:65:TRP:N	1.76	0.83
1:H:152:MET:HG2	1:H:176:PHE:HD1	1.44	0.83
1:B:100:ARG:HG3	1:B:100:ARG:HH11	1.42	0.82
1:D:72:THR:HG22	1:D:322:LYS:HB3	1.61	0.82
1:G:79:TRP:HZ2	1:G:98:ILE:CD1	1.90	0.82
1:F:82:LEU:HD13	1:F:98:ILE:HD11	1.60	0.81
1:I:81:GLU:HG2	1:I:316:VAL:HG23	1.61	0.81
1:A:88:LYS:HA	1:A:90:ARG:N	1.96	0.81
1:I:65:TRP:HB2	1:I:178:ALA:O	1.80	0.81
1:A:72:THR:HG21	1:B:109:LYS:NZ	1.96	0.80
1:B:330:PRO:C	1:C:143:ARG:HH22	1.89	0.80
1:C:94:LEU:HD13	1:C:214:LYS:HG3	1.63	0.80
1:H:66:THR:OG1	1:H:177:THR:HB	1.80	0.80
1:I:181:SER:OG	1:I:330:PRO:HD2	1.81	0.80
1:D:181:SER:OG	1:D:330:PRO:HD2	1.82	0.79
1:C:135:LYS:CB	1:C:138:GLU:HB3	2.14	0.78
1:D:122:ARG:HA	1:D:128:MET:HE3	1.63	0.78
1:G:80:GLN:HA	1:G:80:GLN:HE21	1.49	0.77
1:C:124:SER:HB3	1:C:127:VAL:HG12	1.67	0.77
1:E:208:ARG:HG2	1:E:313:ILE:HG21	1.67	0.77
1:D:65:TRP:HD1	1:D:179:PRO:O	1.66	0.76
1:B:238:GLN:O	1:B:242:TYR:HD2	1.69	0.76
1:A:237:ILE:HD11	1:A:285:GLU:HB3	1.68	0.76
1:F:226:ARG:HG2	1:F:298:LEU:HD21	1.66	0.76
1:A:213:ILE:HG23	1:I:87:THR:HG21	1.65	0.75
1:B:330:PRO:C	1:C:143:ARG:NH2	2.45	0.75
1:C:138:GLU:O	1:C:140:ASP:N	2.19	0.75
1:I:111:PHE:CZ	1:I:174:LEU:HD23	2.22	0.75
1:F:65:TRP:N	1:F:65:TRP:CE3	2.54	0.75
1:B:219:LYS:HG2	1:B:305:VAL:CG1	2.17	0.74
1:B:222:LEU:HD12	1:B:223:ALA:N	2.02	0.74
1:A:109:LYS:NZ	1:I:72:THR:HG21	2.02	0.74
1:F:180:THR:HG23	1:F:183:GLU:CB	2.17	0.74
1:C:96:ILE:HD12	1:C:207:VAL:HG13	1.70	0.73
1:E:182:GLU:O	1:E:186:THR:HG23	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:111:PHE:CE1	1:I:174:LEU:HD23	2.23	0.73
1:E:85:THR:HG23	1:E:313:ILE:HD11	1.70	0.73
1:F:98:ILE:HD12	1:F:98:ILE:O	1.86	0.73
1:B:181:SER:HB2	1:B:330:PRO:HG2	1.69	0.73
1:D:99:ASP:HB3	1:D:102:GLU:HB2	1.71	0.73
1:F:284:ILE:HD12	1:G:242:TYR:CD1	2.24	0.73
1:B:106:LEU:HD23	1:B:199:VAL:HG22	1.70	0.73
1:B:169:TYR:CD2	1:C:109:LYS:HD2	2.24	0.73
1:H:139:LEU:HD23	1:H:139:LEU:O	1.88	0.73
1:E:92:LEU:HD23	1:E:308:LEU:HD12	1.71	0.72
1:G:98:ILE:C	1:G:98:ILE:HD12	2.14	0.72
1:F:127:VAL:HG12	1:F:128:MET:HE2	1.70	0.72
1:E:200:VAL:HB	1:E:318:PHE:CE2	2.24	0.71
1:C:86:PHE:CZ	1:C:98:ILE:HG13	2.20	0.71
1:G:77:VAL:HG11	1:H:202:GLU:HG3	1.71	0.71
1:A:88:LYS:HA	1:A:89:LEU:C	2.15	0.71
1:A:232:GLN:NE2	1:I:296:GLY:HA3	2.06	0.70
1:G:280:ARG:HG3	1:G:280:ARG:NH1	1.90	0.70
1:F:92:LEU:HD23	1:F:308:LEU:HD23	1.70	0.70
1:H:94:LEU:HD22	1:H:96:ILE:CG2	2.21	0.70
1:H:106:LEU:HD23	1:H:199:VAL:HG23	1.72	0.70
1:C:233:LEU:HD11	1:C:288:VAL:HG11	1.74	0.70
1:E:127:VAL:HG12	1:E:128:MET:HE2	1.72	0.70
1:F:284:ILE:HD12	1:G:242:TYR:CE1	2.26	0.70
1:A:72:THR:HG21	1:B:109:LYS:HZ1	1.55	0.69
1:B:301:ARG:HH11	1:B:301:ARG:CG	1.95	0.69
1:A:72:THR:HG23	1:A:322:LYS:HB3	1.74	0.69
1:B:100:ARG:HH11	1:B:100:ARG:CG	2.05	0.69
1:D:153:LYS:HD2	1:D:154:ALA:N	2.04	0.69
1:C:85:THR:HG21	1:C:313:ILE:HG23	1.74	0.68
1:G:229:MET:HE1	1:G:298:LEU:HD21	1.75	0.68
1:F:300:ASN:O	1:F:303:TYR:HB3	1.93	0.68
1:G:229:MET:CE	1:G:298:LEU:HD11	2.23	0.68
1:G:244:LEU:HD13	1:G:278:ILE:HG22	1.74	0.68
1:C:237:ILE:HD11	1:C:285:GLU:O	1.94	0.68
1:C:139:LEU:C	1:C:139:LEU:HD12	2.18	0.68
1:C:117:LEU:HD13	1:C:149:SER:HB2	1.74	0.68
1:E:208:ARG:HG2	1:E:313:ILE:HG22	1.75	0.68
1:G:79:TRP:CE2	1:G:98:ILE:HD11	2.28	0.68
1:A:325:LEU:HD13	1:B:114:VAL:HB	1.74	0.68
1:C:89:LEU:HD11	1:C:313:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:LYS:HG3	1:E:246:ILE:HD13	1.76	0.67
1:A:80:GLN:OE1	1:B:209:ASN:HB3	1.95	0.67
1:B:252:ILE:HD12	1:B:271:ILE:HG21	1.77	0.67
1:A:88:LYS:CA	1:A:90:ARG:N	2.57	0.67
1:H:199:VAL:CG1	1:H:320:PRO:HG3	2.24	0.67
1:C:121:LEU:HD22	1:C:127:VAL:HG21	1.75	0.67
1:D:85:THR:HA	1:D:88:LYS:HZ3	1.60	0.67
1:I:307:GLN:HA	1:I:307:GLN:NE2	2.10	0.67
1:A:192:ILE:HD11	1:A:323:TYR:OH	1.95	0.66
1:E:117:LEU:HD11	1:E:152:MET:HB2	1.77	0.66
1:D:178:ALA:HB1	1:D:179:PRO:HD2	1.78	0.66
1:C:72:THR:CG2	1:C:322:LYS:HB3	2.24	0.66
1:D:240:LEU:HB3	1:D:282:LEU:HD13	1.77	0.66
1:C:87:THR:HG22	1:C:90:ARG:HH12	1.60	0.66
1:H:225:ASP:OD2	1:H:301:ARG:NH2	2.29	0.66
1:A:70:VAL:H	1:A:325:LEU:HB3	1.61	0.66
1:D:329:LEU:HD12	1:D:330:PRO:HD2	1.76	0.66
1:C:255:PRO:HG3	1:D:252:ILE:HD11	1.78	0.66
1:I:139:LEU:HA	1:I:141:LEU:HD21	1.78	0.65
1:I:208:ARG:NH2	1:I:313:ILE:O	2.29	0.65
1:A:66:THR:OG1	1:A:177:THR:HB	1.96	0.65
1:A:234:ASP:OD2	1:I:299:ARG:CZ	2.44	0.65
1:C:240:LEU:HD23	1:C:282:LEU:HA	1.78	0.65
1:F:158:ASN:OD1	1:F:158:ASN:C	2.39	0.65
1:A:182:GLU:O	1:A:186:THR:HG23	1.96	0.65
1:E:183:GLU:O	1:E:187:VAL:HG23	1.96	0.65
1:D:65:TRP:CD1	1:D:179:PRO:O	2.50	0.65
1:C:296:GLY:HA3	1:D:232:GLN:OE1	1.95	0.65
1:F:95:ASP:O	1:F:96:ILE:HD13	1.97	0.64
1:I:83:GLU:O	1:I:87:THR:HG23	1.96	0.64
1:A:244:LEU:HD13	1:A:278:ILE:HG22	1.79	0.64
1:E:85:THR:HG21	1:E:313:ILE:HD11	1.79	0.64
1:B:100:ARG:HG3	1:B:100:ARG:NH1	2.04	0.64
1:B:72:THR:HG22	1:B:322:LYS:HB3	1.78	0.64
1:G:65:TRP:HB2	1:G:179:PRO:O	1.98	0.64
1:H:96:ILE:O	1:H:96:ILE:HG13	1.98	0.64
1:F:182:GLU:N	1:F:182:GLU:OE1	2.31	0.64
1:D:285:GLU:O	1:D:288:VAL:HG12	1.98	0.64
1:G:86:PHE:HZ	1:G:98:ILE:HG23	1.61	0.64
1:H:152:MET:HG2	1:H:176:PHE:CD1	2.31	0.64
1:B:219:LYS:HG2	1:B:305:VAL:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ASP:O	1:D:158:ASN:CB	2.45	0.63
1:G:280:ARG:CG	1:G:280:ARG:NH1	2.54	0.63
1:I:282:LEU:O	1:I:286:LYS:HG3	1.99	0.63
1:A:87:THR:O	1:A:87:THR:HG23	1.98	0.63
1:E:329:LEU:HB3	1:F:142:HIS:HE2	1.64	0.63
1:F:307:GLN:HE22	1:G:224:GLN:HG3	1.63	0.63
1:D:76:PRO:HG3	1:D:100:ARG:HH12	1.63	0.63
1:D:107:PHE:CD1	1:D:195:ILE:HG22	2.34	0.63
1:E:280:ARG:HD2	1:E:283:GLU:OE2	1.99	0.63
1:A:152:MET:HE1	1:A:188:LEU:HA	1.79	0.62
1:F:180:THR:CG2	1:F:183:GLU:HB3	2.29	0.62
1:D:73:PRO:HD3	1:D:170:THR:HG22	1.81	0.62
1:F:218:GLU:HA	1:F:218:GLU:OE1	1.98	0.62
1:C:135:LYS:CB	1:C:138:GLU:OE1	2.47	0.62
1:F:199:VAL:HG21	1:F:320:PRO:HG3	1.81	0.62
1:C:124:SER:CB	1:C:127:VAL:HG12	2.29	0.62
1:C:233:LEU:HD11	1:C:288:VAL:CG1	2.29	0.62
1:F:204:ILE:HD12	1:F:205:GLU:N	2.14	0.62
1:I:117:LEU:HD23	1:I:191:TYR:CE1	2.34	0.62
1:C:87:THR:HG22	1:C:90:ARG:NH1	2.14	0.62
1:E:178:ALA:HB1	1:E:179:PRO:HD2	1.81	0.62
1:A:109:LYS:HZ3	1:I:72:THR:HG21	1.65	0.62
1:F:284:ILE:HG23	1:G:242:TYR:CD1	2.35	0.62
1:G:86:PHE:CE2	1:G:96:ILE:HG22	2.36	0.61
1:A:180:THR:HG22	1:A:181:SER:H	1.65	0.61
1:F:325:LEU:HA	1:G:115:SER:OG	2.00	0.61
1:C:182:GLU:O	1:C:186:THR:HG23	2.00	0.61
1:E:296:GLY:HA3	1:F:232:GLN:OE1	2.01	0.61
1:B:94:LEU:HD22	1:B:96:ILE:HG12	1.82	0.61
1:D:240:LEU:HD21	1:D:281:LYS:HB3	1.82	0.61
1:I:99:ASP:HB3	1:I:102:GLU:HG3	1.83	0.61
1:C:168:LEU:C	1:C:168:LEU:HD12	2.26	0.61
1:B:219:LYS:HG2	1:B:305:VAL:HG11	1.83	0.61
1:C:168:LEU:CD1	1:C:169:TYR:HD2	2.13	0.60
1:A:94:LEU:CG	1:A:214:LYS:HD2	2.21	0.60
1:E:96:ILE:C	1:E:96:ILE:HD12	2.26	0.60
1:C:124:SER:HB3	1:C:127:VAL:CG1	2.30	0.60
1:H:282:LEU:O	1:H:282:LEU:HD23	2.01	0.60
1:H:67:SER:HB2	1:H:184:ALA:HB1	1.82	0.60
1:D:281:LYS:HG3	1:E:246:ILE:CD1	2.31	0.60
1:F:200:VAL:HG22	1:F:318:PHE:CE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ASP:C	1:D:156:ASP:OD1	2.42	0.60
1:A:79:TRP:HZ2	1:A:98:ILE:HG22	1.65	0.60
1:C:240:LEU:HB3	1:C:282:LEU:HD13	1.84	0.60
1:C:156:ASP:HB2	1:C:172:TRP:CE2	2.36	0.59
1:E:240:LEU:HD23	1:E:282:LEU:HA	1.83	0.59
1:C:144:ALA:O	1:C:147:ALA:HB3	2.02	0.59
1:I:307:GLN:HA	1:I:307:GLN:HE21	1.65	0.59
1:D:329:LEU:HD12	1:D:330:PRO:CD	2.32	0.59
1:E:65:TRP:HD1	1:E:179:PRO:O	1.85	0.59
1:E:85:THR:HG22	1:E:86:PHE:N	2.16	0.59
1:F:72:THR:HG21	1:G:109:LYS:NZ	2.16	0.59
1:G:229:MET:HE1	1:G:298:LEU:HD11	1.84	0.59
1:B:225:ASP:OD2	1:B:301:ARG:NH2	2.36	0.59
1:H:174:LEU:HD11	1:H:192:ILE:HD11	1.85	0.59
1:A:244:LEU:HD21	1:A:279:GLU:HG3	1.84	0.59
1:D:76:PRO:HG3	1:D:100:ARG:NH1	2.16	0.59
1:F:284:ILE:CG2	1:G:242:TYR:HD1	2.16	0.59
1:I:301:ARG:HH21	1:I:301:ARG:CG	1.96	0.59
1:B:252:ILE:HD12	1:B:271:ILE:CG2	2.33	0.59
1:G:98:ILE:HD12	1:G:98:ILE:O	2.02	0.59
1:H:128:MET:HE1	1:H:145:ILE:HD11	1.85	0.59
1:B:226:ARG:HH22	1:B:290:ASP:HB2	1.67	0.59
1:D:212:GLU:OE1	1:D:212:GLU:HA	2.03	0.59
1:D:222:LEU:HD13	1:D:301:ARG:CB	2.32	0.58
1:I:98:ILE:HD13	1:I:203:SER:HB3	1.85	0.58
1:D:77:VAL:HG21	1:E:202:GLU:OE1	2.04	0.58
1:I:72:THR:HG22	1:I:73:PRO:O	2.03	0.58
1:G:302:GLN:O	1:G:306:GLU:HG3	2.03	0.58
1:I:74:PRO:HD3	1:I:320:PRO:O	2.03	0.58
1:E:82:LEU:CD2	1:E:316:VAL:HG11	2.33	0.58
1:I:298:LEU:O	1:I:298:LEU:HD23	2.04	0.58
1:D:120:TYR:OH	1:D:190:GLY:HA3	2.04	0.58
1:C:96:ILE:CD1	1:C:207:VAL:HG13	2.34	0.58
1:D:140:ASP:OD1	1:D:140:ASP:N	2.35	0.58
1:G:96:ILE:HG21	1:G:207:VAL:HG13	1.85	0.58
1:H:199:VAL:HG13	1:H:320:PRO:HG3	1.86	0.58
1:I:140:ASP:OD1	1:I:140:ASP:C	2.46	0.58
1:D:216:GLN:O	1:D:216:GLN:HG2	2.04	0.58
1:H:199:VAL:HG11	1:H:320:PRO:HG3	1.86	0.58
1:A:94:LEU:HD22	1:A:96:ILE:HG23	1.87	0.57
1:B:200:VAL:HG23	1:B:318:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:THR:HG22	1:A:181:SER:N	2.19	0.57
1:G:79:TRP:CZ2	1:G:98:ILE:CD1	2.71	0.57
1:E:243:SER:OG	1:E:269:PHE:HB3	2.04	0.57
1:F:226:ARG:CG	1:F:298:LEU:HD21	2.34	0.57
1:G:86:PHE:CZ	1:G:98:ILE:HG23	2.39	0.57
1:H:240:LEU:HD21	1:H:281:LYS:HG2	1.87	0.57
1:A:156:ASP:C	1:A:157:ASP:OD2	2.47	0.57
1:C:77:VAL:HG11	1:D:202:GLU:OE2	2.05	0.57
1:D:139:LEU:O	1:D:139:LEU:HD12	2.04	0.57
1:E:282:LEU:HD13	1:E:282:LEU:C	2.29	0.57
1:F:204:ILE:HD13	1:F:208:ARG:HH21	1.69	0.57
1:C:74:PRO:HG3	1:C:320:PRO:C	2.30	0.57
1:D:86:PHE:N	1:D:86:PHE:CD2	2.72	0.57
1:F:89:LEU:HD11	1:F:313:ILE:HD11	1.86	0.57
1:H:96:ILE:CD1	1:H:207:VAL:HG13	2.34	0.57
1:H:254:LYS:O	1:H:255:PRO:O	2.23	0.57
1:A:111:PHE:CZ	1:A:174:LEU:HD22	2.40	0.57
1:B:303:TYR:OH	1:C:227:ILE:HD12	2.05	0.57
1:H:122:ARG:HA	1:H:128:MET:HE3	1.86	0.57
1:A:79:TRP:CZ2	1:A:98:ILE:HG22	2.39	0.56
1:A:252:ILE:HD11	1:A:256:VAL:HG23	1.87	0.56
1:B:152:MET:HE1	1:B:188:LEU:HA	1.85	0.56
1:B:185:GLN:HB2	1:B:328:SER:O	2.04	0.56
1:C:139:LEU:O	1:C:141:LEU:N	2.38	0.56
1:F:72:THR:HG22	1:F:322:LYS:HB3	1.87	0.56
1:H:67:SER:HB2	1:H:184:ALA:CB	2.36	0.56
1:H:74:PRO:HG3	1:H:321:PHE:N	2.19	0.56
1:I:142:HIS:O	1:I:146:VAL:HG23	2.05	0.56
1:D:86:PHE:N	1:D:86:PHE:HD2	2.02	0.56
1:A:111:PHE:CE2	1:A:174:LEU:HD22	2.41	0.56
1:D:86:PHE:CZ	1:D:98:ILE:HG13	2.40	0.56
1:G:282:LEU:HD11	1:G:286:LYS:HE2	1.87	0.56
1:I:307:GLN:HE21	1:I:307:GLN:CA	2.19	0.56
1:B:240:LEU:HD23	1:B:282:LEU:HA	1.86	0.56
1:C:79:TRP:CE2	1:C:100:ARG:HG2	2.41	0.56
1:F:192:ILE:HG21	1:F:323:TYR:OH	2.06	0.56
1:A:76:PRO:HG3	1:A:100:ARG:HH12	1.71	0.56
1:F:181:SER:HB3	1:F:182:GLU:OE1	2.06	0.56
1:H:77:VAL:HG21	1:I:202:GLU:HG3	1.87	0.56
1:F:152:MET:HE1	1:F:188:LEU:HD12	1.88	0.56
1:D:280:ARG:HH11	1:D:283:GLU:HG3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:OD2	1:A:268:ASP:N	2.39	0.55
1:B:106:LEU:HD23	1:B:199:VAL:CG2	2.36	0.55
1:E:117:LEU:HD13	1:E:149:SER:HA	1.88	0.55
1:I:199:VAL:HG11	1:I:320:PRO:HG2	1.87	0.55
1:B:238:GLN:O	1:B:242:TYR:CD2	2.55	0.55
1:I:180:THR:HG22	1:I:181:SER:H	1.72	0.55
1:B:156:ASP:HB2	1:B:172:TRP:CE2	2.42	0.55
1:F:199:VAL:CG2	1:F:320:PRO:HG3	2.37	0.55
1:I:120:TYR:CE2	1:I:191:TYR:HB2	2.42	0.55
1:A:329:LEU:HD12	1:A:330:PRO:HD2	1.88	0.55
1:G:86:PHE:CD2	1:G:96:ILE:HG22	2.42	0.55
1:E:85:THR:CG2	1:E:86:PHE:N	2.70	0.55
1:F:124:SER:O	1:F:128:MET:HG2	2.07	0.55
1:I:119:GLU:O	1:I:123:SER:HB3	2.06	0.55
1:A:70:VAL:HG12	1:A:324:GLN:HB2	1.88	0.55
1:I:152:MET:HE1	1:I:188:LEU:HA	1.87	0.55
1:D:114:VAL:O	1:D:118:GLU:HG3	2.07	0.55
1:F:65:TRP:HB3	1:F:178:ALA:O	2.06	0.55
1:C:279:GLU:O	1:C:283:GLU:HG2	2.07	0.54
1:F:207:VAL:HG12	1:F:313:ILE:HG13	1.88	0.54
1:B:169:TYR:CG	1:C:109:LYS:HD2	2.42	0.54
1:E:117:LEU:HD11	1:E:152:MET:CB	2.35	0.54
1:F:256:VAL:O	1:F:256:VAL:HG23	2.07	0.54
1:E:247:ALA:N	1:E:271:ILE:HD11	2.23	0.54
1:C:253:LYS:O	1:C:276:ASP:OD2	2.26	0.54
1:D:111:PHE:C	1:D:113:SER:H	2.15	0.54
1:F:309:THR:O	1:F:309:THR:HG22	2.07	0.54
1:A:88:LYS:CA	1:A:90:ARG:H	2.21	0.54
1:A:157:ASP:OD2	1:A:157:ASP:N	2.41	0.54
1:F:153:LYS:HG3	1:F:175:SER:OG	2.08	0.54
1:H:74:PRO:HG3	1:H:320:PRO:C	2.33	0.54
1:D:255:PRO:HG2	1:E:252:ILE:HD11	1.90	0.54
1:A:232:GLN:CD	1:I:296:GLY:HA3	2.33	0.54
1:B:229:MET:HG3	1:B:298:LEU:HD11	1.89	0.54
1:C:71:VAL:HG13	1:C:104:PHE:HE1	1.72	0.54
1:C:168:LEU:HD12	1:C:169:TYR:HD2	1.72	0.54
1:H:253:LYS:NZ	1:H:276:ASP:CB	2.70	0.54
1:A:196:SER:HA	1:A:199:VAL:CG1	2.38	0.54
1:C:266:ASP:HB3	1:C:270:SER:HA	1.89	0.53
1:A:244:LEU:HD13	1:A:278:ILE:CG2	2.37	0.53
1:G:126:TYR:OH	1:G:183:GLU:HG2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:LEU:HD12	1:H:174:LEU:O	2.08	0.53
1:B:94:LEU:HG	1:B:214:LYS:HG2	1.89	0.53
1:D:86:PHE:CE1	1:D:98:ILE:HG13	2.44	0.53
1:H:89:LEU:HD21	1:H:313:ILE:HD11	1.90	0.53
1:A:199:VAL:HG11	1:A:320:PRO:HG3	1.91	0.53
1:G:152:MET:HE1	1:G:188:LEU:HA	1.89	0.53
1:B:76:PRO:HA	1:B:100:ARG:HE	1.72	0.53
1:D:117:LEU:HD21	1:D:152:MET:HG3	1.89	0.53
1:G:293:GLU:HA	1:G:299:ARG:HH21	1.73	0.53
1:A:239:ARG:HH12	1:I:294:LEU:HB3	1.73	0.53
1:A:88:LYS:CB	1:A:91:VAL:HB	2.39	0.53
1:A:284:ILE:HG23	1:B:242:TYR:CD1	2.43	0.53
1:E:74:PRO:HD3	1:E:321:PHE:HA	1.90	0.53
1:E:204:ILE:C	1:E:204:ILE:HD12	2.34	0.53
1:H:96:ILE:HD11	1:H:207:VAL:HG13	1.90	0.53
1:A:239:ARG:NH1	1:I:294:LEU:HB3	2.23	0.53
1:F:66:THR:OG1	1:F:177:THR:HB	2.09	0.52
1:A:80:GLN:HE22	1:B:213:ILE:HD11	1.75	0.52
1:A:256:VAL:HG12	1:A:256:VAL:O	2.09	0.52
1:C:233:LEU:C	1:C:233:LEU:HD23	2.35	0.52
1:C:255:PRO:CG	1:D:252:ILE:HD11	2.39	0.52
1:B:197:ALA:HA	1:B:200:VAL:HG12	1.92	0.52
1:H:196:SER:OG	1:H:320:PRO:HD2	2.09	0.52
1:I:96:ILE:HD11	1:I:210:LYS:HD3	1.92	0.52
1:C:168:LEU:HD12	1:C:169:TYR:CD2	2.45	0.52
1:D:89:LEU:HD11	1:D:313:ILE:HD11	1.91	0.52
1:F:284:ILE:CG2	1:G:242:TYR:CD1	2.93	0.52
1:I:81:GLU:HG2	1:I:316:VAL:CG2	2.37	0.52
1:A:71:VAL:HG13	1:A:104:PHE:HE1	1.74	0.52
1:E:214:LYS:HG3	1:E:308:LEU:HD21	1.92	0.52
1:H:204:ILE:HD12	1:H:205:GLU:N	2.24	0.52
1:I:66:THR:O	1:I:66:THR:HG22	2.09	0.52
1:A:252:ILE:HG12	1:A:252:ILE:O	2.08	0.52
1:I:301:ARG:O	1:I:305:VAL:HG23	2.10	0.52
1:A:255:PRO:HG3	1:B:252:ILE:HD11	1.92	0.52
1:B:237:ILE:HD11	1:B:285:GLU:O	2.09	0.52
1:C:181:SER:HB2	1:C:330:PRO:HD2	1.91	0.52
1:F:152:MET:HE1	1:F:188:LEU:CD1	2.40	0.52
1:G:71:VAL:HG12	1:G:71:VAL:O	2.09	0.52
1:D:106:LEU:HD21	1:D:110:LYS:NZ	2.24	0.52
1:E:299:ARG:NH1	1:F:234:ASP:HB3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:LEU:HD23	1:G:199:VAL:CG2	2.29	0.52
1:I:72:THR:HG23	1:I:73:PRO:HD2	1.92	0.52
1:A:109:LYS:HZ1	1:I:72:THR:HG21	1.71	0.51
1:D:107:PHE:CE1	1:D:195:ILE:HG22	2.45	0.51
1:E:229:MET:HG3	1:E:298:LEU:HD11	1.92	0.51
1:A:76:PRO:HG3	1:A:100:ARG:NH1	2.26	0.51
1:C:131:LEU:CB	1:C:141:LEU:HD21	2.40	0.51
1:E:75:GLU:CG	1:E:322:LYS:HD2	2.40	0.51
1:E:94:LEU:HD22	1:E:96:ILE:CG2	2.40	0.51
1:E:117:LEU:HD11	1:E:152:MET:HG3	1.91	0.51
1:F:117:LEU:HD21	1:F:152:MET:HB2	1.93	0.51
1:F:74:PRO:O	1:F:100:ARG:HD2	2.11	0.51
1:G:117:LEU:HD21	1:G:152:MET:HB2	1.92	0.51
1:H:72:THR:HB	1:H:73:PRO:CD	2.40	0.51
1:D:323:TYR:CE2	1:D:327:PRO:HD3	2.46	0.51
1:G:82:LEU:HB3	1:G:86:PHE:CE1	2.45	0.51
1:H:156:ASP:OD1	1:H:157:ASP:N	2.44	0.51
1:I:326:SER:O	1:I:327:PRO:C	2.54	0.51
1:D:65:TRP:HB2	1:D:178:ALA:O	2.11	0.51
1:E:75:GLU:HG2	1:E:322:LYS:HD2	1.93	0.51
1:E:126:TYR:C	1:E:126:TYR:CD2	2.88	0.51
1:E:130:GLN:N	1:E:130:GLN:OE1	2.44	0.51
1:A:284:ILE:CG2	1:B:242:TYR:CD1	2.94	0.51
1:E:106:LEU:O	1:E:110:LYS:HG2	2.11	0.51
1:F:204:ILE:HD12	1:F:205:GLU:HG2	1.93	0.51
1:I:139:LEU:HA	1:I:141:LEU:CD2	2.40	0.51
1:A:199:VAL:CG1	1:A:320:PRO:HG3	2.41	0.51
1:B:93:ASP:CG	1:B:93:ASP:O	2.54	0.51
1:D:86:PHE:HD2	1:D:86:PHE:H	1.59	0.51
1:F:321:PHE:CD1	1:F:321:PHE:C	2.89	0.51
1:G:289:THR:HG22	1:G:290:ASP:N	2.25	0.51
1:A:282:LEU:HD22	1:A:286:LYS:HE3	1.91	0.50
1:I:200:VAL:HG22	1:I:318:PHE:CE2	2.47	0.50
1:A:98:ILE:HG22	1:A:98:ILE:O	2.10	0.50
1:F:72:THR:HG21	1:G:109:LYS:HZ3	1.75	0.50
1:H:94:LEU:HD22	1:H:96:ILE:HG23	1.93	0.50
1:H:180:THR:HB	1:H:183:GLU:HB2	1.92	0.50
1:H:300:ASN:O	1:H:303:TYR:HB3	2.11	0.50
1:I:307:GLN:NE2	1:I:307:GLN:CA	2.73	0.50
1:I:150:GLU:O	1:I:153:LYS:HE2	2.11	0.50
1:I:220:GLU:OE1	1:I:220:GLU:HA	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ARG:HD2	1:C:128:MET:CE	2.42	0.50
1:G:65:TRP:C	1:G:65:TRP:CD1	2.90	0.50
1:E:180:THR:OG1	1:E:183:GLU:HB2	2.12	0.50
1:F:280:ARG:NH1	1:G:249:ALA:HB2	2.27	0.50
1:A:117:LEU:HD13	1:A:191:TYR:CZ	2.47	0.50
1:C:218:GLU:OE1	1:C:218:GLU:HA	2.12	0.50
1:E:117:LEU:HD11	1:E:152:MET:CG	2.41	0.50
1:F:88:LYS:O	1:F:92:LEU:HD13	2.11	0.50
1:C:87:THR:HG21	1:D:213:ILE:HG23	1.94	0.50
1:E:299:ARG:HH12	1:F:234:ASP:HB3	1.77	0.50
1:H:174:LEU:CD1	1:H:192:ILE:HD11	2.41	0.50
1:H:219:LYS:HG3	1:H:220:GLU:N	2.20	0.50
1:B:99:ASP:HB3	1:B:102:GLU:HB2	1.95	0.49
1:C:135:LYS:HA	1:C:138:GLU:HB3	1.94	0.49
1:D:110:LYS:O	1:D:113:SER:HB3	2.12	0.49
1:A:266:ASP:CG	1:A:267:PRO:HD2	2.38	0.49
1:C:156:ASP:HB2	1:C:172:TRP:CZ2	2.47	0.49
1:I:182:GLU:O	1:I:186:THR:HG23	2.12	0.49
1:A:270:SER:O	1:A:271:ILE:HD12	2.12	0.49
1:A:96:ILE:HD11	1:A:207:VAL:HG13	1.94	0.49
1:A:200:VAL:HG12	1:A:318:PHE:CE2	2.47	0.49
1:B:70:VAL:HG23	1:B:325:LEU:HB3	1.95	0.49
1:E:66:THR:HG22	1:E:177:THR:HG1	1.74	0.49
1:A:195:ILE:O	1:A:199:VAL:HG12	2.12	0.49
1:B:80:GLN:OE1	1:C:209:ASN:HB3	2.12	0.49
1:B:215:THR:OG1	1:B:308:LEU:HB3	2.13	0.49
1:F:73:PRO:HA	1:F:104:PHE:CD1	2.48	0.49
1:B:240:LEU:HB3	1:B:282:LEU:HD23	1.94	0.49
1:D:117:LEU:CD2	1:D:152:MET:HG3	2.43	0.49
1:F:237:ILE:HD13	1:F:286:LYS:HG2	1.95	0.48
1:C:122:ARG:HD2	1:C:128:MET:HE3	1.95	0.48
1:D:280:ARG:NH1	1:D:283:GLU:HG3	2.28	0.48
1:E:225:ASP:CB	1:E:301:ARG:HH12	2.25	0.48
1:C:75:GLU:OE2	1:D:109:LYS:NZ	2.46	0.48
1:F:129:ASP:OD1	1:F:130:GLN:N	2.45	0.48
1:F:275:ALA:HA	1:F:278:ILE:HB	1.95	0.48
1:I:319:THR:HG22	1:I:321:PHE:H	1.79	0.48
1:F:127:VAL:HG12	1:F:128:MET:CE	2.42	0.48
1:A:80:GLN:OE1	1:B:209:ASN:CB	2.61	0.48
1:C:80:GLN:O	1:C:84:LYS:HG3	2.13	0.48
1:A:111:PHE:HE1	1:A:192:ILE:HG22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:O	1:A:284:ILE:HD12	2.13	0.48
1:C:113:SER:HB3	1:C:116:LEU:HB2	1.96	0.48
1:G:295:ASN:O	1:G:299:ARG:HG3	2.14	0.48
1:C:168:LEU:C	1:C:168:LEU:CD1	2.87	0.48
1:E:91:VAL:HG21	1:F:220:GLU:HB3	1.96	0.48
1:F:142:HIS:O	1:F:146:VAL:HG23	2.14	0.48
1:F:329:LEU:HB3	1:G:142:HIS:NE2	2.29	0.48
1:I:204:ILE:HG22	1:I:205:GLU:N	2.28	0.48
1:A:268:ASP:HB2	1:A:269:PHE:CD1	2.49	0.48
1:C:134:ALA:O	1:C:135:LYS:CB	2.61	0.48
1:D:323:TYR:CD2	1:D:326:SER:HA	2.49	0.48
1:F:284:ILE:HG23	1:G:242:TYR:CE1	2.49	0.48
1:I:156:ASP:C	1:I:158:ASN:H	2.21	0.48
1:C:74:PRO:HG3	1:C:321:PHE:N	2.29	0.48
1:D:196:SER:O	1:D:200:VAL:HG13	2.13	0.48
1:E:329:LEU:HB3	1:F:142:HIS:NE2	2.28	0.48
1:G:199:VAL:HG13	1:G:320:PRO:HG3	1.96	0.48
1:I:226:ARG:HG2	1:I:298:LEU:HD11	1.96	0.48
1:C:87:THR:C	1:C:89:LEU:N	2.70	0.47
1:C:89:LEU:HD12	1:C:96:ILE:HD11	1.96	0.47
1:C:135:LYS:CA	1:C:138:GLU:HB3	2.44	0.47
1:E:141:LEU:O	1:E:144:ALA:HB3	2.14	0.47
1:H:96:ILE:O	1:H:96:ILE:CG1	2.61	0.47
1:E:269:PHE:CD1	1:E:269:PHE:N	2.81	0.47
1:F:70:VAL:HG13	1:F:325:LEU:HB3	1.96	0.47
1:F:289:THR:HG22	1:F:290:ASP:N	2.28	0.47
1:F:180:THR:CG2	1:F:183:GLU:CB	2.90	0.47
1:G:93:ASP:O	1:G:93:ASP:CG	2.57	0.47
1:H:295:ASN:HB3	1:H:298:LEU:HB2	1.95	0.47
1:A:213:ILE:CG2	1:I:87:THR:HG21	2.39	0.47
1:A:237:ILE:CD1	1:A:285:GLU:HB3	2.39	0.47
1:B:254:LYS:HD3	1:B:254:LYS:N	2.30	0.47
1:E:196:SER:O	1:E:199:VAL:HG13	2.15	0.47
1:F:233:LEU:HD22	1:F:291:VAL:HG12	1.96	0.47
1:I:256:VAL:O	1:I:256:VAL:HG23	2.13	0.47
1:A:222:LEU:O	1:A:226:ARG:HG3	2.14	0.47
1:B:199:VAL:HG11	1:B:320:PRO:HG3	1.96	0.47
1:E:216:GLN:HG2	1:E:216:GLN:O	2.14	0.47
1:B:85:THR:HG22	1:B:86:PHE:N	2.29	0.47
1:B:66:THR:O	1:B:330:PRO:HB3	2.15	0.47
1:C:139:LEU:HD12	1:C:139:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:LEU:HG	1:E:277:GLY:HA3	1.95	0.47
1:H:300:ASN:OD1	1:I:228:LYS:HA	2.15	0.47
1:E:279:GLU:O	1:E:279:GLU:HG2	2.15	0.46
1:E:313:ILE:O	1:E:313:ILE:HG23	2.15	0.46
1:G:178:ALA:HB1	1:G:179:PRO:HD2	1.96	0.46
1:G:204:ILE:HD11	1:G:316:VAL:O	2.15	0.46
1:H:94:LEU:HD22	1:H:96:ILE:HG21	1.97	0.46
1:A:267:PRO:HG2	1:A:268:ASP:OD2	2.15	0.46
1:B:319:THR:C	1:B:321:PHE:H	2.22	0.46
1:D:72:THR:CG2	1:D:322:LYS:HB3	2.39	0.46
1:E:185:GLN:HB2	1:E:328:SER:O	2.15	0.46
1:A:66:THR:OG1	1:A:177:THR:CB	2.63	0.46
1:B:229:MET:HE2	1:B:229:MET:HA	1.97	0.46
1:E:85:THR:HG23	1:E:313:ILE:CD1	2.42	0.46
1:F:295:ASN:N	1:F:295:ASN:OD1	2.47	0.46
1:B:271:ILE:O	1:B:272:SER:C	2.57	0.46
1:C:85:THR:CG2	1:C:313:ILE:HG23	2.45	0.46
1:G:72:THR:HB	1:G:73:PRO:HD2	1.96	0.46
1:E:121:LEU:O	1:E:128:MET:HE3	2.15	0.46
1:F:72:THR:HG23	1:F:73:PRO:O	2.16	0.46
1:H:114:VAL:O	1:H:118:GLU:HG3	2.15	0.46
1:C:99:ASP:HB3	1:C:102:GLU:HB2	1.96	0.46
1:E:128:MET:HE2	1:E:128:MET:HA	1.98	0.46
1:F:82:LEU:HD23	1:F:82:LEU:HA	1.71	0.46
1:A:284:ILE:HG23	1:B:242:TYR:CE1	2.50	0.46
1:B:75:GLU:HB3	1:B:76:PRO:HD2	1.98	0.46
1:A:72:THR:HG21	1:B:109:LYS:HZ3	1.74	0.46
1:B:75:GLU:OE2	1:C:109:LYS:NZ	2.49	0.46
1:B:253:LYS:C	1:B:254:LYS:HD3	2.39	0.46
1:C:285:GLU:O	1:C:288:VAL:HG12	2.16	0.46
1:H:71:VAL:HG13	1:H:104:PHE:HE1	1.81	0.46
1:I:117:LEU:HD23	1:I:191:TYR:CD1	2.50	0.46
1:D:195:ILE:O	1:D:199:VAL:HG23	2.16	0.46
1:F:79:TRP:CZ2	1:F:98:ILE:CD1	2.99	0.46
1:I:222:LEU:HD13	1:I:301:ARG:HB3	1.97	0.46
1:C:135:LYS:CB	1:C:138:GLU:CB	2.88	0.45
1:I:199:VAL:HG11	1:I:320:PRO:CG	2.45	0.45
1:I:321:PHE:CD1	1:I:321:PHE:C	2.94	0.45
1:B:204:ILE:HD13	1:B:204:ILE:HA	1.81	0.45
1:B:278:ILE:O	1:B:282:LEU:HB2	2.15	0.45
1:F:66:THR:HA	1:F:177:THR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:VAL:CG1	1:F:325:LEU:HB3	2.46	0.45
1:A:66:THR:O	1:A:66:THR:HG22	2.16	0.45
1:A:90:ARG:HA	1:A:94:LEU:O	2.17	0.45
1:F:307:GLN:NE2	1:G:224:GLN:HG3	2.31	0.45
1:C:116:LEU:HD23	1:C:116:LEU:HA	1.69	0.45
1:A:176:PHE:HB3	1:A:188:LEU:HB2	1.98	0.45
1:G:250:ALA:HB3	1:G:252:ILE:HG13	1.98	0.45
1:H:83:GLU:O	1:H:87:THR:OG1	2.34	0.45
1:G:95:ASP:O	1:G:96:ILE:HD13	2.17	0.45
1:I:141:LEU:HD23	1:I:141:LEU:N	2.22	0.45
1:B:272:SER:O	1:B:274:GLY:N	2.49	0.45
1:A:80:GLN:NE2	1:B:213:ILE:HD11	2.32	0.45
1:C:92:LEU:O	1:C:93:ASP:OD1	2.35	0.45
1:C:242:TYR:O	1:C:246:ILE:HD12	2.17	0.45
1:E:178:ALA:HB1	1:E:179:PRO:CD	2.46	0.45
1:E:314:ASN:O	1:E:316:VAL:N	2.50	0.45
1:A:245:ASP:HB3	1:I:280:ARG:HE	1.82	0.44
1:B:242:TYR:O	1:B:246:ILE:HG13	2.17	0.44
1:F:156:ASP:O	1:F:158:ASN:N	2.44	0.44
1:F:222:LEU:HD13	1:F:301:ARG:HB3	2.00	0.44
1:A:128:MET:HA	1:A:128:MET:HE2	2.00	0.44
1:D:85:THR:HG21	1:D:313:ILE:HG23	1.99	0.44
1:F:329:LEU:HD23	1:G:142:HIS:CD2	2.52	0.44
1:H:66:THR:O	1:H:66:THR:HG22	2.17	0.44
1:I:266:ASP:HA	1:I:267:PRO:HD3	1.85	0.44
1:D:111:PHE:O	1:D:113:SER:N	2.50	0.44
1:D:141:LEU:O	1:D:145:ILE:HG12	2.17	0.44
1:E:80:GLN:OE1	1:F:209:ASN:HB3	2.16	0.44
1:A:91:VAL:C	1:A:93:ASP:H	2.25	0.44
1:C:111:PHE:CZ	1:C:174:LEU:HD22	2.52	0.44
1:C:181:SER:CB	1:C:330:PRO:HD2	2.48	0.44
1:C:271:ILE:O	1:C:272:SER:C	2.60	0.44
1:A:87:THR:CG2	1:B:216:GLN:NE2	2.81	0.44
1:A:282:LEU:O	1:A:286:LYS:HG3	2.18	0.44
1:E:282:LEU:HD13	1:E:282:LEU:O	2.18	0.44
1:F:284:ILE:HG21	1:G:242:TYR:HD1	1.82	0.44
1:H:253:LYS:HZ3	1:H:276:ASP:CB	2.31	0.44
1:I:94:LEU:HG	1:I:214:LYS:HG3	1.99	0.44
1:D:116:LEU:HD23	1:D:116:LEU:HA	1.89	0.44
1:E:280:ARG:HA	1:E:283:GLU:HG2	1.99	0.44
1:F:156:ASP:OD2	1:F:158:ASN:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HD13	1:A:191:TYR:CE2	2.53	0.44
1:D:255:PRO:HA	1:D:272:SER:O	2.17	0.44
1:G:98:ILE:CD1	1:G:98:ILE:C	2.84	0.44
1:H:150:GLU:O	1:H:153:LYS:NZ	2.51	0.44
1:A:238:GLN:HB3	1:I:294:LEU:HD23	1.99	0.44
1:D:66:THR:OG1	1:D:177:THR:HB	2.17	0.44
1:I:92:LEU:HD23	1:I:308:LEU:HD23	2.00	0.44
1:I:117:LEU:HA	1:I:191:TYR:CE1	2.53	0.44
1:A:105:ASN:ND2	1:I:168:LEU:HD11	2.33	0.44
1:B:139:LEU:C	1:B:141:LEU:H	2.24	0.44
1:D:194:TYR:HD2	1:D:195:ILE:HD13	1.82	0.44
1:A:100:ARG:HE	1:A:100:ARG:HB2	1.37	0.43
1:A:152:MET:O	1:A:153:LYS:HD3	2.18	0.43
1:B:246:ILE:HG22	1:B:271:ILE:HD11	1.98	0.43
1:D:119:GLU:O	1:D:119:GLU:OE2	2.36	0.43
1:H:180:THR:HG22	1:H:181:SER:N	2.34	0.43
1:B:156:ASP:HB2	1:B:172:TRP:CZ2	2.53	0.43
1:E:268:ASP:HB3	1:E:269:PHE:CD1	2.53	0.43
1:F:117:LEU:CD2	1:F:152:MET:HB2	2.48	0.43
1:H:92:LEU:HG	1:H:308:LEU:HD13	2.00	0.43
1:A:65:TRP:HA	1:A:178:ALA:O	2.18	0.43
1:A:185:GLN:O	1:A:189:SER:HB2	2.18	0.43
1:C:319:THR:C	1:C:321:PHE:H	2.26	0.43
1:E:198:LEU:HD12	1:E:198:LEU:HA	1.68	0.43
1:H:298:LEU:HD22	1:H:298:LEU:HA	1.74	0.43
1:B:128:MET:O	1:B:129:ASP:C	2.60	0.43
1:B:281:LYS:C	1:B:283:GLU:N	2.76	0.43
1:C:139:LEU:C	1:C:139:LEU:CD1	2.84	0.43
1:C:295:ASN:OD1	1:C:298:LEU:HG	2.18	0.43
1:E:92:LEU:HD21	1:E:307:GLN:HB3	2.00	0.43
1:A:121:LEU:HB3	1:A:145:ILE:HD12	2.00	0.43
1:C:65:TRP:N	1:C:181:SER:HA	2.34	0.43
1:D:65:TRP:HA	1:D:65:TRP:CE3	2.54	0.43
1:E:280:ARG:HE	1:F:245:ASP:HB3	1.84	0.43
1:E:310:LYS:O	1:E:311:ALA:C	2.62	0.43
1:D:89:LEU:HD11	1:D:313:ILE:CD1	2.48	0.43
1:G:92:LEU:HD12	1:G:92:LEU:HA	1.86	0.43
1:G:98:ILE:CD1	1:G:98:ILE:O	2.66	0.43
1:G:181:SER:O	1:G:184:ALA:HB3	2.19	0.43
1:H:152:MET:HE1	1:H:188:LEU:HA	2.01	0.43
1:C:87:THR:C	1:C:89:LEU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:PHE:CD2	1:H:108:ILE:HD13	2.53	0.43
1:H:185:GLN:O	1:H:186:THR:C	2.60	0.43
1:D:178:ALA:HB1	1:D:179:PRO:CD	2.47	0.43
1:F:72:THR:OG1	1:F:73:PRO:HD2	2.18	0.43
1:F:256:VAL:O	1:F:256:VAL:CG2	2.66	0.43
1:G:92:LEU:O	1:G:93:ASP:OD1	2.37	0.43
1:I:301:ARG:NH2	1:I:301:ARG:CG	2.66	0.43
1:A:87:THR:C	1:A:88:LYS:O	2.61	0.42
1:F:284:ILE:HD13	1:F:284:ILE:HA	1.86	0.42
1:G:92:LEU:HG	1:G:308:LEU:HD13	2.01	0.42
1:I:193:ASP:O	1:I:194:TYR:C	2.62	0.42
1:A:212:GLU:O	1:A:212:GLU:HG2	2.18	0.42
1:C:88:LYS:HE2	1:C:312:ASN:O	2.19	0.42
1:C:290:ASP:OD1	1:C:290:ASP:C	2.63	0.42
1:D:73:PRO:CD	1:D:170:THR:HG22	2.49	0.42
1:E:65:TRP:HA	1:E:65:TRP:CE3	2.53	0.42
1:G:319:THR:HA	1:G:320:PRO:HD3	1.90	0.42
1:A:229:MET:HE2	1:A:229:MET:HB2	1.53	0.42
1:C:90:ARG:HG3	1:C:95:ASP:OD1	2.19	0.42
1:H:252:ILE:O	1:H:252:ILE:HG22	2.18	0.42
1:A:92:LEU:HB3	1:A:308:LEU:CD1	2.49	0.42
1:B:197:ALA:O	1:B:200:VAL:HG12	2.18	0.42
1:B:199:VAL:HG11	1:B:320:PRO:HB3	2.02	0.42
1:D:290:ASP:C	1:D:290:ASP:OD1	2.61	0.42
1:F:204:ILE:CD1	1:F:205:GLU:HG2	2.50	0.42
1:G:152:MET:SD	1:G:176:PHE:HB2	2.60	0.42
1:G:208:ARG:NH2	1:G:315:ASP:OD1	2.50	0.42
1:H:255:PRO:C	1:H:256:VAL:HG12	2.44	0.42
1:H:255:PRO:HG2	1:I:252:ILE:HD11	2.01	0.42
1:A:87:THR:HG23	1:B:216:GLN:NE2	2.33	0.42
1:A:142:HIS:O	1:A:146:VAL:HG23	2.19	0.42
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.83	0.42
1:D:111:PHE:C	1:D:113:SER:N	2.76	0.42
1:A:92:LEU:HD23	1:A:308:LEU:HD12	2.00	0.42
1:A:301:ARG:HE	1:A:301:ARG:HB2	1.67	0.42
1:C:70:VAL:HG23	1:C:325:LEU:HD23	2.01	0.42
1:C:168:LEU:HD11	1:C:169:TYR:HD2	1.82	0.42
1:I:110:LYS:O	1:I:113:SER:HB3	2.20	0.42
1:A:86:PHE:CE2	1:A:97:LYS:HA	2.54	0.42
1:B:255:PRO:CG	1:C:252:ILE:HD11	2.32	0.42
1:B:305:VAL:O	1:B:305:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:THR:HG23	1:C:73:PRO:O	2.19	0.42
1:C:213:ILE:HD13	1:C:213:ILE:HA	1.92	0.42
1:D:221:LYS:HB3	1:D:301:ARG:NH2	2.35	0.42
1:H:222:LEU:O	1:H:223:ALA:C	2.62	0.42
1:I:92:LEU:HB3	1:I:308:LEU:HD21	2.01	0.42
1:C:168:LEU:CD1	1:C:169:TYR:CD2	2.99	0.42
1:D:198:LEU:HD12	1:D:198:LEU:HA	1.73	0.42
1:D:280:ARG:NH1	1:D:284:ILE:HG13	2.35	0.42
1:F:65:TRP:HD1	1:F:179:PRO:O	2.03	0.42
1:G:199:VAL:CG1	1:G:320:PRO:HG3	2.50	0.42
1:B:92:LEU:HD23	1:B:308:LEU:HD12	2.02	0.42
1:E:82:LEU:HD23	1:E:316:VAL:HG11	2.01	0.42
1:E:94:LEU:HD22	1:E:96:ILE:HG23	2.01	0.42
1:I:76:PRO:HD3	1:I:100:ARG:CZ	2.49	0.42
1:A:96:ILE:HD12	1:A:207:VAL:HG22	2.02	0.42
1:A:198:LEU:HD12	1:A:198:LEU:HA	1.77	0.42
1:C:266:ASP:HA	1:C:267:PRO:HD3	1.80	0.42
1:E:192:ILE:HG21	1:E:323:TYR:OH	2.19	0.42
1:H:253:LYS:HZ1	1:H:276:ASP:CB	2.32	0.42
1:A:79:TRP:HZ2	1:A:98:ILE:CG2	2.32	0.41
1:A:290:ASP:OD1	1:A:290:ASP:C	2.63	0.41
1:C:81:GLU:H	1:C:81:GLU:HG2	1.39	0.41
1:C:246:ILE:HG22	1:C:271:ILE:HG21	2.02	0.41
1:E:65:TRP:HA	1:E:65:TRP:HE3	1.85	0.41
1:E:117:LEU:O	1:E:121:LEU:HG	2.20	0.41
1:F:282:LEU:O	1:F:286:LYS:HG3	2.20	0.41
1:I:286:LYS:HE2	1:I:286:LYS:HB3	1.80	0.41
1:A:87:THR:O	1:A:87:THR:CG2	2.66	0.41
1:E:65:TRP:HB2	1:E:178:ALA:O	2.20	0.41
1:F:121:LEU:O	1:F:128:MET:HE3	2.20	0.41
1:F:204:ILE:HD12	1:F:204:ILE:C	2.45	0.41
1:F:240:LEU:HD12	1:F:240:LEU:HA	1.90	0.41
1:G:98:ILE:HD13	1:G:103:ALA:HB2	2.02	0.41
1:H:85:THR:HG21	1:H:313:ILE:HG23	2.01	0.41
1:H:117:LEU:HD11	1:H:152:MET:HB2	2.02	0.41
1:C:106:LEU:HD23	1:C:199:VAL:HG13	2.02	0.41
1:C:156:ASP:OD2	1:C:157:ASP:N	2.53	0.41
1:E:215:THR:HA	1:E:308:LEU:HD23	2.01	0.41
1:E:314:ASN:O	1:E:315:ASP:C	2.63	0.41
1:F:140:ASP:O	1:F:141:LEU:C	2.62	0.41
1:G:290:ASP:OD1	1:G:290:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:VAL:HG12	1:F:71:VAL:O	2.20	0.41
1:G:77:VAL:HG11	1:H:202:GLU:CG	2.47	0.41
1:G:116:LEU:HD23	1:G:116:LEU:HA	1.87	0.41
1:H:92:LEU:O	1:H:93:ASP:CB	2.69	0.41
1:H:303:TYR:OH	1:I:227:ILE:HD12	2.20	0.41
1:B:185:GLN:O	1:B:189:SER:HB2	2.20	0.41
1:G:86:PHE:O	1:G:90:ARG:HB2	2.21	0.41
1:G:222:LEU:O	1:G:223:ALA:C	2.64	0.41
1:I:96:ILE:HD12	1:I:96:ILE:HA	1.58	0.41
1:A:73:PRO:HG3	1:A:104:PHE:CG	2.55	0.41
1:D:81:GLU:HG2	1:D:316:VAL:HG13	2.01	0.41
1:G:222:LEU:HD13	1:G:301:ARG:HB2	2.02	0.41
1:A:111:PHE:CD2	1:A:111:PHE:C	2.99	0.41
1:A:218:GLU:OE2	1:A:218:GLU:HA	2.21	0.41
1:F:192:ILE:HG21	1:F:323:TYR:HH	1.86	0.41
1:H:72:THR:HB	1:H:73:PRO:HD2	2.02	0.41
1:B:319:THR:O	1:B:321:PHE:N	2.53	0.41
1:C:94:LEU:HG	1:C:96:ILE:HG23	2.02	0.41
1:G:122:ARG:HA	1:G:128:MET:HE3	2.01	0.41
1:B:79:TRP:CG	1:B:100:ARG:HD3	2.56	0.41
1:B:219:LYS:CG	1:B:305:VAL:HG13	2.46	0.41
1:D:174:LEU:HD12	1:D:192:ILE:HD11	2.01	0.41
1:E:203:SER:O	1:E:206:ASN:HB2	2.20	0.41
1:F:229:MET:HG3	1:F:298:LEU:CD1	2.50	0.41
1:G:65:TRP:C	1:G:65:TRP:HD1	2.29	0.41
1:H:144:ALA:O	1:H:147:ALA:HB3	2.21	0.41
1:I:184:ALA:O	1:I:185:GLN:C	2.63	0.41
1:B:107:PHE:HD2	1:B:108:ILE:HD13	1.85	0.41
1:E:96:ILE:C	1:E:96:ILE:CD1	2.92	0.41
1:F:79:TRP:HE1	1:F:98:ILE:HD12	1.86	0.41
1:F:94:LEU:HA	1:F:94:LEU:HD23	1.86	0.41
1:F:145:ILE:HD13	1:F:145:ILE:HA	1.94	0.41
1:G:128:MET:O	1:G:129:ASP:C	2.64	0.41
1:A:153:LYS:HD3	1:A:153:LYS:HA	1.85	0.40
1:C:229:MET:HG3	1:C:298:LEU:HD11	2.01	0.40
1:C:244:LEU:HA	1:C:244:LEU:HD12	1.86	0.40
1:D:76:PRO:CG	1:D:100:ARG:NH1	2.83	0.40
1:F:129:ASP:CG	1:F:130:GLN:N	2.78	0.40
1:H:87:THR:HG23	1:H:90:ARG:NH1	2.35	0.40
1:I:290:ASP:OD1	1:I:290:ASP:C	2.64	0.40
1:A:252:ILE:HD13	1:A:271:ILE:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ASP:HB3	1:C:102:GLU:CB	2.51	0.40
1:C:143:ARG:HD3	1:C:143:ARG:HA	1.31	0.40
1:F:71:VAL:HG13	1:F:104:PHE:HE1	1.85	0.40
1:F:215:THR:O	1:F:219:LYS:HB3	2.21	0.40
1:A:252:ILE:HD11	1:A:256:VAL:CG2	2.51	0.40
1:C:139:LEU:O	1:C:140:ASP:C	2.64	0.40
1:F:202:GLU:O	1:F:206:ASN:HB2	2.21	0.40
1:F:275:ALA:O	1:F:279:GLU:HB2	2.20	0.40
1:I:65:TRP:C	1:I:65:TRP:CE3	2.99	0.40
1:I:140:ASP:OD1	1:I:140:ASP:O	2.39	0.40
1:I:196:SER:HA	1:I:199:VAL:HG12	2.03	0.40
1:A:73:PRO:HG3	1:A:104:PHE:CD2	2.56	0.40
1:A:178:ALA:HB1	1:A:179:PRO:HD2	2.02	0.40
1:A:326:SER:O	1:A:327:PRO:C	2.64	0.40
1:B:199:VAL:CG1	1:B:320:PRO:HG3	2.52	0.40
1:C:117:LEU:HD11	1:C:152:MET:HB2	2.02	0.40
1:E:282:LEU:HD11	1:E:286:LYS:NZ	2.36	0.40
1:E:318:PHE:CD2	1:E:318:PHE:N	2.90	0.40
1:H:204:ILE:HD12	1:H:204:ILE:C	2.47	0.40
1:C:79:TRP:O	1:C:82:LEU:N	2.53	0.40
1:D:86:PHE:CE1	1:D:96:ILE:HG22	2.56	0.40
1:E:240:LEU:HD21	1:E:281:LYS:HG2	2.03	0.40
1:F:158:ASN:OD1	1:F:158:ASN:O	2.38	0.40
1:H:304:LEU:O	1:H:305:VAL:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	232/271 (86%)	211 (91%)	17 (7%)	4 (2%)	7 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	232/271 (86%)	212 (91%)	14 (6%)	6 (3%)	4	15
1	C	238/271 (88%)	214 (90%)	18 (8%)	6 (2%)	4	16
1	D	232/271 (86%)	215 (93%)	14 (6%)	3 (1%)	9	31
1	E	233/271 (86%)	212 (91%)	18 (8%)	3 (1%)	9	31
1	F	236/271 (87%)	212 (90%)	23 (10%)	1 (0%)	30	60
1	G	232/271 (86%)	214 (92%)	15 (6%)	3 (1%)	9	31
1	H	234/271 (86%)	219 (94%)	14 (6%)	1 (0%)	30	60
1	I	234/271 (86%)	214 (92%)	16 (7%)	4 (2%)	7	25
All	All	2103/2439 (86%)	1923 (91%)	149 (7%)	31 (2%)	8	28

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	255	PRO
1	C	139	LEU
1	C	140	ASP
1	D	112	GLN
1	D	255	PRO
1	D	315	ASP
1	E	255	PRO
1	E	315	ASP
1	G	179	PRO
1	H	255	PRO
1	I	255	PRO
1	A	88	LYS
1	A	272	SER
1	B	273	LEU
1	B	275	ALA
1	I	315	ASP
1	A	89	LEU
1	B	272	SER
1	B	315	ASP
1	C	272	SER
1	I	129	ASP
1	C	141	LEU
1	G	223	ALA
1	B	278	ILE
1	C	179	PRO
1	F	157	ASP

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Mol	Chain	Res	Type
1	G	315	ASP
1	I	76	PRO
1	C	252	ILE
1	E	91	VAL
1	A	267	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	204/243 (84%)	162 (79%)	42 (21%)	1 4
1	B	210/243 (86%)	178 (85%)	32 (15%)	3 10
1	C	197/243 (81%)	160 (81%)	37 (19%)	1 5
1	D	198/243 (82%)	169 (85%)	29 (15%)	3 11
1	E	196/243 (81%)	164 (84%)	32 (16%)	2 8
1	F	201/243 (83%)	174 (87%)	27 (13%)	4 13
1	G	198/243 (82%)	166 (84%)	32 (16%)	2 8
1	H	196/243 (81%)	169 (86%)	27 (14%)	3 12
1	I	200/243 (82%)	168 (84%)	32 (16%)	2 9
All	All	1800/2187 (82%)	1510 (84%)	290 (16%)	2 8

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	71	VAL
1	A	79	TRP
1	A	81	GLU
1	A	92	LEU
1	A	94	LEU
1	A	98	ILE
1	A	100	ARG
1	A	101	THR

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Mol	Chain	Res	Type
1	A	109	LYS
1	A	121	LEU
1	A	130	GLN
1	A	141	LEU
1	A	151	LYS
1	A	157	ASP
1	A	167	SER
1	A	171	SER
1	A	186	THR
1	A	192	ILE
1	A	198	LEU
1	A	199	VAL
1	A	206	ASN
1	A	210	LYS
1	A	215	THR
1	A	229	MET
1	A	234	ASP
1	A	237	ILE
1	A	238	GLN
1	A	252	ILE
1	A	268	ASP
1	A	271	ILE
1	A	278	ILE
1	A	279	GLU
1	A	282	LEU
1	A	284	ILE
1	A	288	VAL
1	A	289	THR
1	A	291	VAL
1	A	298	LEU
1	A	301	ARG
1	A	308	LEU
1	A	326	SER
1	B	72	THR
1	B	79	TRP
1	B	85	THR
1	B	87	THR
1	B	92	LEU
1	B	93	ASP
1	B	94	LEU
1	B	96	ILE
1	B	100	ARG

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Mol	Chain	Res	Type
1	B	124	SER
1	B	127	VAL
1	B	130	GLN
1	B	140	ASP
1	B	153	LYS
1	B	177	THR
1	B	189	SER
1	B	198	LEU
1	B	199	VAL
1	B	204	ILE
1	B	211	LEU
1	B	222	LEU
1	B	227	ILE
1	B	233	LEU
1	B	243	SER
1	B	244	LEU
1	B	252	ILE
1	B	283	GLU
1	B	297	GLU
1	B	301	ARG
1	B	308	LEU
1	B	310	LYS
1	B	326	SER
1	C	71	VAL
1	C	72	THR
1	C	77	VAL
1	C	79	TRP
1	C	81	GLU
1	C	82	LEU
1	C	92	LEU
1	C	93	ASP
1	C	117	LEU
1	C	128	MET
1	C	138	GLU
1	C	139	LEU
1	C	143	ARG
1	C	168	LEU
1	C	177	THR
1	C	180	THR
1	C	181	SER
1	C	182	GLU
1	C	186	THR

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Mol	Chain	Res	Type
1	C	189	SER
1	C	198	LEU
1	C	204	ILE
1	C	206	ASN
1	C	210	LYS
1	C	214	LYS
1	C	224	GLN
1	C	233	LEU
1	C	246	ILE
1	C	252	ILE
1	C	271	ILE
1	C	276	ASP
1	C	284	ILE
1	C	289	THR
1	C	302	GLN
1	C	312	ASN
1	C	315	ASP
1	C	317	ASN
1	D	72	THR
1	D	77	VAL
1	D	79	TRP
1	D	86	PHE
1	D	87	THR
1	D	88	LYS
1	D	92	LEU
1	D	96	ILE
1	D	101	THR
1	D	139	LEU
1	D	140	ASP
1	D	153	LYS
1	D	170	THR
1	D	177	THR
1	D	182	GLU
1	D	195	ILE
1	D	198	LEU
1	D	200	VAL
1	D	203	SER
1	D	205	GLU
1	D	216	GLN
1	D	221	LYS
1	D	229	MET
1	D	238	GLN

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Mol	Chain	Res	Type
1	D	241	ASN
1	D	256	VAL
1	D	289	THR
1	D	297	GLU
1	D	308	LEU
1	E	71	VAL
1	E	72	THR
1	E	77	VAL
1	E	85	THR
1	E	87	THR
1	E	91	VAL
1	E	92	LEU
1	E	94	LEU
1	E	96	ILE
1	E	117	LEU
1	E	129	ASP
1	E	139	LEU
1	E	145	ILE
1	E	155	VAL
1	E	180	THR
1	E	186	THR
1	E	189	SER
1	E	198	LEU
1	E	199	VAL
1	E	200	VAL
1	E	203	SER
1	E	204	ILE
1	E	213	ILE
1	E	216	GLN
1	E	256	VAL
1	E	282	LEU
1	E	288	VAL
1	E	291	VAL
1	E	309	THR
1	E	312	ASN
1	E	316	VAL
1	E	325	LEU
1	F	65	TRP
1	F	66	THR
1	F	70	VAL
1	F	71	VAL
1	F	72	THR

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Mol	Chain	Res	Type
1	F	94	LEU
1	F	101	THR
1	F	141	LEU
1	F	158	ASN
1	F	177	THR
1	F	198	LEU
1	F	199	VAL
1	F	206	ASN
1	F	211	LEU
1	F	214	LYS
1	F	232	GLN
1	F	237	ILE
1	F	252	ILE
1	F	256	VAL
1	F	283	GLU
1	F	284	ILE
1	F	285	GLU
1	F	289	THR
1	F	294	LEU
1	F	298	LEU
1	F	316	VAL
1	F	327	PRO
1	G	65	TRP
1	G	71	VAL
1	G	77	VAL
1	G	79	TRP
1	G	80	GLN
1	G	81	GLU
1	G	87	THR
1	G	92	LEU
1	G	93	ASP
1	G	94	LEU
1	G	96	ILE
1	G	97	LYS
1	G	98	ILE
1	G	101	THR
1	G	119	GLU
1	G	130	GLN
1	G	141	LEU
1	G	177	THR
1	G	180	THR
1	G	198	LEU

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Mol	Chain	Res	Type
1	G	228	LYS
1	G	229	MET
1	G	238	GLN
1	G	241	ASN
1	G	256	VAL
1	G	271	ILE
1	G	272	SER
1	G	278	ILE
1	G	280	ARG
1	G	289	THR
1	G	301	ARG
1	G	308	LEU
1	H	66	THR
1	H	71	VAL
1	H	79	TRP
1	H	87	THR
1	H	92	LEU
1	H	94	LEU
1	H	115	SER
1	H	117	LEU
1	H	123	SER
1	H	129	ASP
1	H	149	SER
1	H	153	LYS
1	H	177	THR
1	H	182	GLU
1	H	183	GLU
1	H	198	LEU
1	H	219	LYS
1	H	224	GLN
1	H	232	GLN
1	H	256	VAL
1	H	271	ILE
1	H	291	VAL
1	H	298	LEU
1	H	301	ARG
1	H	308	LEU
1	H	314	ASN
1	H	322	LYS
1	I	65	TRP
1	I	66	THR
1	I	72	THR

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Mol	Chain	Res	Type
1	I	76	PRO
1	I	77	VAL
1	I	79	TRP
1	I	88	LYS
1	I	89	LEU
1	I	92	LEU
1	I	94	LEU
1	I	96	ILE
1	I	117	LEU
1	I	130	GLN
1	I	141	LEU
1	I	177	THR
1	I	186	THR
1	I	199	VAL
1	I	201	LYS
1	I	204	ILE
1	I	206	ASN
1	I	213	ILE
1	I	214	LYS
1	I	220	GLU
1	I	221	LYS
1	I	256	VAL
1	I	268	ASP
1	I	291	VAL
1	I	295	ASN
1	I	301	ARG
1	I	307	GLN
1	I	316	VAL
1	I	317	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	130	GLN
1	A	142	HIS
1	A	185	GLN
1	A	224	GLN
1	A	324	GLN
1	B	185	GLN
1	B	216	GLN
1	D	307	GLN

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Mol	Chain	Res	Type
1	E	142	HIS
1	E	324	GLN
1	F	307	GLN
1	F	324	GLN
1	G	80	GLN
1	G	130	GLN
1	G	224	GLN
1	G	314	ASN
1	G	324	GLN
1	H	232	GLN
1	H	241	ASN
1	I	142	HIS
1	I	295	ASN
1	I	307	GLN
1	I	314	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](#)

There are no ligands in this entry.

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	240/271 (88%)	0.66	15 (6%) 26 19	41, 56, 74, 88	0
1	B	240/271 (88%)	0.63	17 (7%) 22 16	44, 60, 77, 89	0
1	C	246/271 (90%)	0.79	28 (11%) 10 7	44, 64, 80, 89	0
1	D	240/271 (88%)	0.79	19 (7%) 18 13	43, 62, 82, 95	0
1	E	241/271 (88%)	0.72	15 (6%) 26 20	41, 61, 80, 94	0
1	F	244/271 (90%)	0.61	16 (6%) 24 18	38, 58, 78, 89	0
1	G	240/271 (88%)	0.54	16 (6%) 24 17	40, 56, 76, 94	0
1	H	242/271 (89%)	0.57	10 (4%) 41 33	42, 56, 75, 97	0
1	I	242/271 (89%)	0.57	13 (5%) 31 24	39, 58, 75, 89	0
All	All	2175/2439 (89%)	0.65	149 (6%) 23 16	38, 59, 79, 97	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	65	TRP	6.3
1	C	130	GLN	5.9
1	F	256	VAL	5.2
1	E	139	LEU	5.1
1	H	130	GLN	5.1
1	D	139	LEU	5.0
1	A	65	TRP	4.8
1	A	139	LEU	4.7
1	B	256	VAL	4.7
1	G	272	SER	4.3
1	H	139	LEU	4.3
1	A	89	LEU	4.2
1	A	256	VAL	4.1
1	C	140	ASP	4.1
1	G	139	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	97	LYS	4.0
1	D	251	GLY	4.0
1	F	139	LEU	4.0
1	C	251	GLY	3.9
1	I	251	GLY	3.9
1	B	139	LEU	3.9
1	I	65	TRP	3.8
1	C	65	TRP	3.7
1	D	256	VAL	3.7
1	C	139	LEU	3.7
1	A	250	ALA	3.7
1	C	266	ASP	3.7
1	E	257	TYR	3.7
1	F	137	ASP	3.6
1	G	129	ASP	3.5
1	G	234	ASP	3.4
1	G	256	VAL	3.4
1	I	139	LEU	3.3
1	I	256	VAL	3.3
1	F	159	ALA	3.3
1	E	130	GLN	3.2
1	A	140	ASP	3.2
1	D	249	ALA	3.1
1	F	285	GLU	3.1
1	E	140	ASP	3.1
1	G	65	TRP	3.1
1	D	252	ILE	3.1
1	H	159	ALA	3.0
1	C	315	ASP	3.0
1	I	293	GLU	3.0
1	I	141	LEU	2.9
1	A	249	ALA	2.9
1	A	180	THR	2.9
1	C	131	LEU	2.9
1	I	93	ASP	2.9
1	C	80	GLN	2.9
1	D	295	ASN	2.9
1	E	142	HIS	2.9
1	B	65	TRP	2.8
1	C	138	GLU	2.8
1	B	212	GLU	2.8
1	C	86	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	158	ASN	2.8
1	F	138	GLU	2.7
1	C	256	VAL	2.7
1	D	316	VAL	2.7
1	C	129	ASP	2.7
1	A	302	GLN	2.7
1	E	314	ASN	2.7
1	H	256	VAL	2.7
1	H	253	LYS	2.6
1	I	287	ALA	2.6
1	F	295	ASN	2.6
1	I	276	ASP	2.6
1	A	88	LYS	2.6
1	B	129	ASP	2.6
1	E	167	SER	2.6
1	I	252	ILE	2.6
1	A	86	PHE	2.6
1	A	85	THR	2.6
1	H	289	THR	2.5
1	B	130	GLN	2.5
1	G	247	ALA	2.5
1	B	234	ASP	2.5
1	F	167	SER	2.5
1	C	96	ILE	2.5
1	F	249	ALA	2.5
1	G	245	ASP	2.4
1	E	329	LEU	2.4
1	A	234	ASP	2.4
1	C	81	GLU	2.4
1	D	86	PHE	2.4
1	D	119	GLU	2.4
1	E	123	SER	2.4
1	C	134	ALA	2.4
1	C	302	GLN	2.4
1	B	276	ASP	2.4
1	G	95	ASP	2.4
1	I	253	LYS	2.4
1	H	167	SER	2.4
1	D	296	GLY	2.3
1	H	129	ASP	2.3
1	G	130	GLN	2.3
1	D	312	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	283	GLU	2.3
1	F	65	TRP	2.3
1	B	96	ILE	2.3
1	C	90	ARG	2.3
1	G	251	GLY	2.3
1	F	266	ASP	2.3
1	E	251	GLY	2.3
1	D	273	LEU	2.3
1	A	287	ALA	2.2
1	D	182	GLU	2.2
1	C	248	ASN	2.2
1	E	141	LEU	2.2
1	G	232	GLN	2.2
1	G	140	ASP	2.2
1	B	141	LEU	2.2
1	E	249	ALA	2.2
1	I	183	GLU	2.2
1	I	129	ASP	2.2
1	C	255	PRO	2.2
1	B	285	GLU	2.2
1	B	297	GLU	2.2
1	G	266	ASP	2.2
1	B	254	LYS	2.2
1	B	81	GLU	2.2
1	D	267	PRO	2.1
1	E	254	LYS	2.1
1	D	272	SER	2.1
1	A	90	ARG	2.1
1	E	226	ARG	2.1
1	F	98	ILE	2.1
1	D	314	ASN	2.1
1	D	268	ASP	2.1
1	C	85	THR	2.1
1	B	249	ALA	2.1
1	C	189	SER	2.1
1	G	96	ILE	2.1
1	C	230	LYS	2.1
1	H	99	ASP	2.1
1	C	249	ALA	2.1
1	F	246	ILE	2.1
1	B	180	THR	2.1
1	C	167	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	97	LYS	2.0
1	C	93	ASP	2.0
1	F	272	SER	2.0
1	G	181	SER	2.0
1	B	267	PRO	2.0
1	E	312	ASN	2.0
1	F	66	THR	2.0
1	D	254	LYS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.