



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:42 PM UTC

PDB ID : 2QGV / pdb_00002qgv
Title : Crystal structure of hydrogenase-1 operon protein hyaE from *Shigella flexneri*.
Northeast Structural Genomics Consortium Target Sfr170
Authors : Forouhar, F.; Su, M.; Seetharaman, J.; Benach, J.; Wang, D.; Fang, Y.; Cunningham, K.; Ma, L.-C.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2007-06-29
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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)

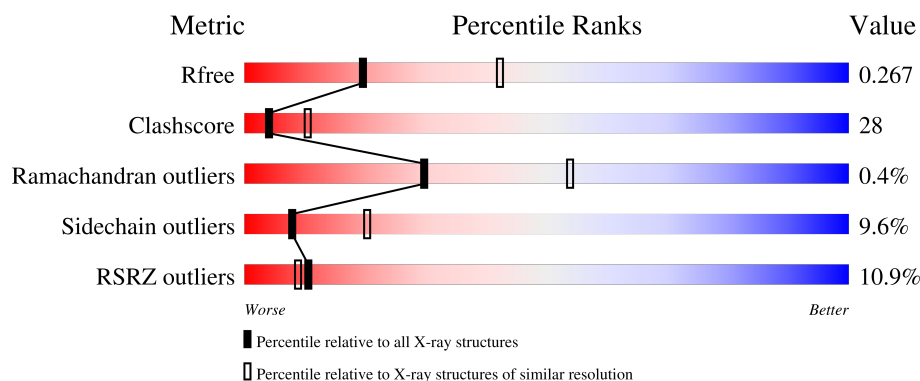
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	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)

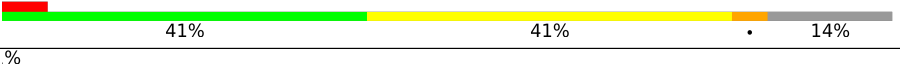
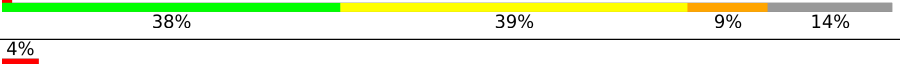
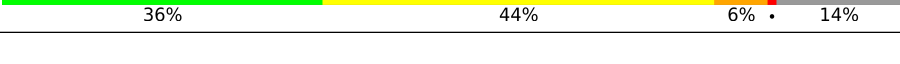
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	140	17% 51% 31% • 14%
1	B	140	13% 49% 34% • 14%
1	C	140	11% 53% 29% • 14%
1	D	140	7% 48% 34% • 14%

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	E	140	
1	F	140	
1	G	140	
1	H	140	
1	I	140	
1	J	140	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9610 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 Hydrogenase-1 operon protein hyaE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	Se	0	0	0
			961	617	163	178	3			
1	B	121	Total	C	N	O	Se	0	0	0
			961	617	163	178	3			
1	C	121	Total	C	N	O	Se	0	0	0
			961	617	163	178	3			
1	D	121	Total	C	N	O	Se	0	0	0
			961	617	163	178	3			
1	E	121	Total	C	N	O	Se	0	0	0
			961	617	163	178	3			
1	F	121	Total	C	N	O	Se	0	0	0
			961	617	163	178	3			
1	G	121	Total	C	N	O	Se	0	0	0
			961	617	163	178	3			
1	H	121	Total	C	N	O	Se	0	0	0
			961	617	163	178	3			
1	I	121	Total	C	N	O	Se	0	0	0
			961	617	163	178	3			
1	J	121	Total	C	N	O	Se	0	0	0
			961	617	163	178	3			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q83RW6
A	14	MSE	MET	modified residue	UNP Q83RW6
A	57	MSE	MET	modified residue	UNP Q83RW6
A	120	MSE	MET	modified residue	UNP Q83RW6
A	133	LEU	-	cloning artifact	UNP Q83RW6
A	134	GLU	-	cloning artifact	UNP Q83RW6
A	135	HIS	-	cloning artifact	UNP Q83RW6
A	136	HIS	-	cloning artifact	UNP Q83RW6
A	137	HIS	-	cloning artifact	UNP Q83RW6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	138	HIS	-	cloning artifact	UNP Q83RW6
A	139	HIS	-	cloning artifact	UNP Q83RW6
A	140	HIS	-	cloning artifact	UNP Q83RW6
B	1	MSE	MET	modified residue	UNP Q83RW6
B	14	MSE	MET	modified residue	UNP Q83RW6
B	57	MSE	MET	modified residue	UNP Q83RW6
B	120	MSE	MET	modified residue	UNP Q83RW6
B	133	LEU	-	cloning artifact	UNP Q83RW6
B	134	GLU	-	cloning artifact	UNP Q83RW6
B	135	HIS	-	cloning artifact	UNP Q83RW6
B	136	HIS	-	cloning artifact	UNP Q83RW6
B	137	HIS	-	cloning artifact	UNP Q83RW6
B	138	HIS	-	cloning artifact	UNP Q83RW6
B	139	HIS	-	cloning artifact	UNP Q83RW6
B	140	HIS	-	cloning artifact	UNP Q83RW6
C	1	MSE	MET	modified residue	UNP Q83RW6
C	14	MSE	MET	modified residue	UNP Q83RW6
C	57	MSE	MET	modified residue	UNP Q83RW6
C	120	MSE	MET	modified residue	UNP Q83RW6
C	133	LEU	-	cloning artifact	UNP Q83RW6
C	134	GLU	-	cloning artifact	UNP Q83RW6
C	135	HIS	-	cloning artifact	UNP Q83RW6
C	136	HIS	-	cloning artifact	UNP Q83RW6
C	137	HIS	-	cloning artifact	UNP Q83RW6
C	138	HIS	-	cloning artifact	UNP Q83RW6
C	139	HIS	-	cloning artifact	UNP Q83RW6
C	140	HIS	-	cloning artifact	UNP Q83RW6
D	1	MSE	MET	modified residue	UNP Q83RW6
D	14	MSE	MET	modified residue	UNP Q83RW6
D	57	MSE	MET	modified residue	UNP Q83RW6
D	120	MSE	MET	modified residue	UNP Q83RW6
D	133	LEU	-	cloning artifact	UNP Q83RW6
D	134	GLU	-	cloning artifact	UNP Q83RW6
D	135	HIS	-	cloning artifact	UNP Q83RW6
D	136	HIS	-	cloning artifact	UNP Q83RW6
D	137	HIS	-	cloning artifact	UNP Q83RW6
D	138	HIS	-	cloning artifact	UNP Q83RW6
D	139	HIS	-	cloning artifact	UNP Q83RW6
D	140	HIS	-	cloning artifact	UNP Q83RW6
E	1	MSE	MET	modified residue	UNP Q83RW6
E	14	MSE	MET	modified residue	UNP Q83RW6
E	57	MSE	MET	modified residue	UNP Q83RW6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	120	MSE	MET	modified residue	UNP Q83RW6
E	133	LEU	-	cloning artifact	UNP Q83RW6
E	134	GLU	-	cloning artifact	UNP Q83RW6
E	135	HIS	-	cloning artifact	UNP Q83RW6
E	136	HIS	-	cloning artifact	UNP Q83RW6
E	137	HIS	-	cloning artifact	UNP Q83RW6
E	138	HIS	-	cloning artifact	UNP Q83RW6
E	139	HIS	-	cloning artifact	UNP Q83RW6
E	140	HIS	-	cloning artifact	UNP Q83RW6
F	1	MSE	MET	modified residue	UNP Q83RW6
F	14	MSE	MET	modified residue	UNP Q83RW6
F	57	MSE	MET	modified residue	UNP Q83RW6
F	120	MSE	MET	modified residue	UNP Q83RW6
F	133	LEU	-	cloning artifact	UNP Q83RW6
F	134	GLU	-	cloning artifact	UNP Q83RW6
F	135	HIS	-	cloning artifact	UNP Q83RW6
F	136	HIS	-	cloning artifact	UNP Q83RW6
F	137	HIS	-	cloning artifact	UNP Q83RW6
F	138	HIS	-	cloning artifact	UNP Q83RW6
F	139	HIS	-	cloning artifact	UNP Q83RW6
F	140	HIS	-	cloning artifact	UNP Q83RW6
G	1	MSE	MET	modified residue	UNP Q83RW6
G	14	MSE	MET	modified residue	UNP Q83RW6
G	57	MSE	MET	modified residue	UNP Q83RW6
G	120	MSE	MET	modified residue	UNP Q83RW6
G	133	LEU	-	cloning artifact	UNP Q83RW6
G	134	GLU	-	cloning artifact	UNP Q83RW6
G	135	HIS	-	cloning artifact	UNP Q83RW6
G	136	HIS	-	cloning artifact	UNP Q83RW6
G	137	HIS	-	cloning artifact	UNP Q83RW6
G	138	HIS	-	cloning artifact	UNP Q83RW6
G	139	HIS	-	cloning artifact	UNP Q83RW6
G	140	HIS	-	cloning artifact	UNP Q83RW6
H	1	MSE	MET	modified residue	UNP Q83RW6
H	14	MSE	MET	modified residue	UNP Q83RW6
H	57	MSE	MET	modified residue	UNP Q83RW6
H	120	MSE	MET	modified residue	UNP Q83RW6
H	133	LEU	-	cloning artifact	UNP Q83RW6
H	134	GLU	-	cloning artifact	UNP Q83RW6
H	135	HIS	-	cloning artifact	UNP Q83RW6
H	136	HIS	-	cloning artifact	UNP Q83RW6
H	137	HIS	-	cloning artifact	UNP Q83RW6

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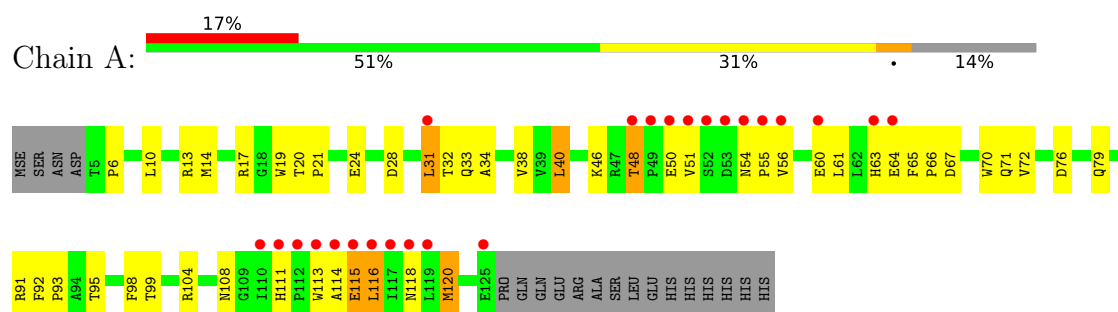
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Chain	Residue	Modelled	Actual	Comment	Reference
H	138	HIS	-	cloning artifact	UNP Q83RW6
H	139	HIS	-	cloning artifact	UNP Q83RW6
H	140	HIS	-	cloning artifact	UNP Q83RW6
I	1	MSE	MET	modified residue	UNP Q83RW6
I	14	MSE	MET	modified residue	UNP Q83RW6
I	57	MSE	MET	modified residue	UNP Q83RW6
I	120	MSE	MET	modified residue	UNP Q83RW6
I	133	LEU	-	cloning artifact	UNP Q83RW6
I	134	GLU	-	cloning artifact	UNP Q83RW6
I	135	HIS	-	cloning artifact	UNP Q83RW6
I	136	HIS	-	cloning artifact	UNP Q83RW6
I	137	HIS	-	cloning artifact	UNP Q83RW6
I	138	HIS	-	cloning artifact	UNP Q83RW6
I	139	HIS	-	cloning artifact	UNP Q83RW6
I	140	HIS	-	cloning artifact	UNP Q83RW6
J	1	MSE	MET	modified residue	UNP Q83RW6
J	14	MSE	MET	modified residue	UNP Q83RW6
J	57	MSE	MET	modified residue	UNP Q83RW6
J	120	MSE	MET	modified residue	UNP Q83RW6
J	133	LEU	-	cloning artifact	UNP Q83RW6
J	134	GLU	-	cloning artifact	UNP Q83RW6
J	135	HIS	-	cloning artifact	UNP Q83RW6
J	136	HIS	-	cloning artifact	UNP Q83RW6
J	137	HIS	-	cloning artifact	UNP Q83RW6
J	138	HIS	-	cloning artifact	UNP Q83RW6
J	139	HIS	-	cloning artifact	UNP Q83RW6
J	140	HIS	-	cloning artifact	UNP Q83RW6

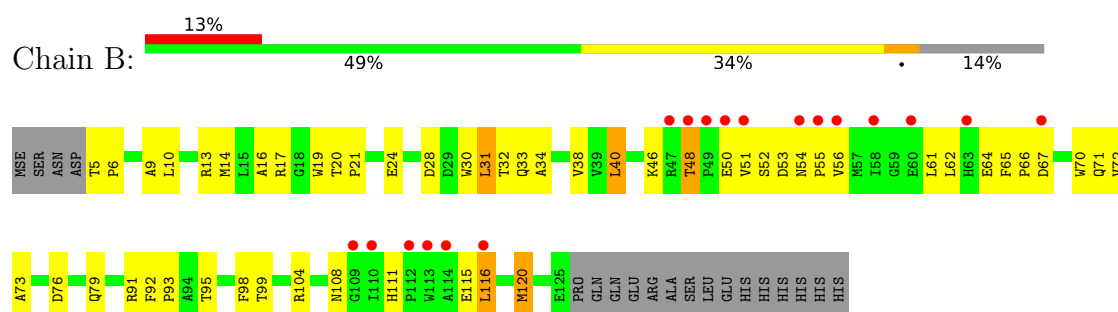
3 Residue-property plots [i](#)

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.

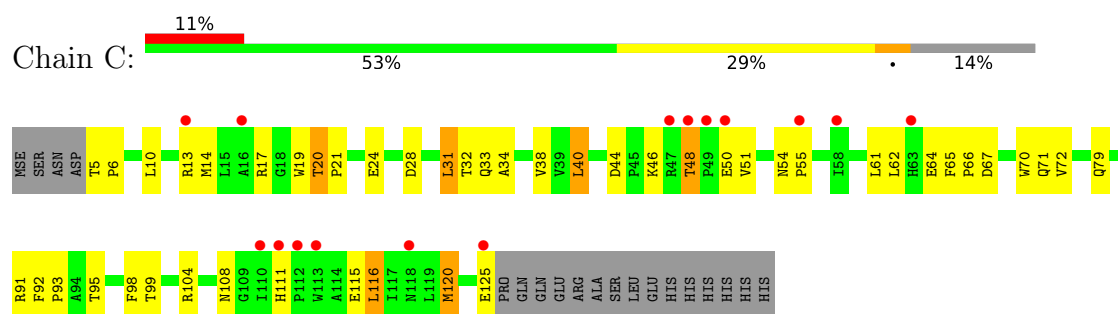
- Molecule 1: Hydrogenase-1 operon protein hyaE



- Molecule 1: Hydrogenase-1 operon protein hyaE



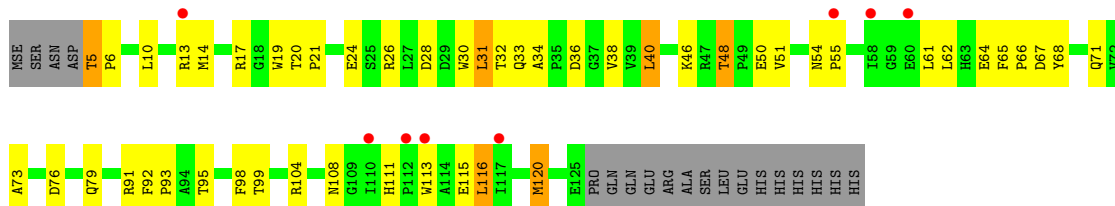
- Molecule 1: Hydrogenase-1 operon protein hyaE



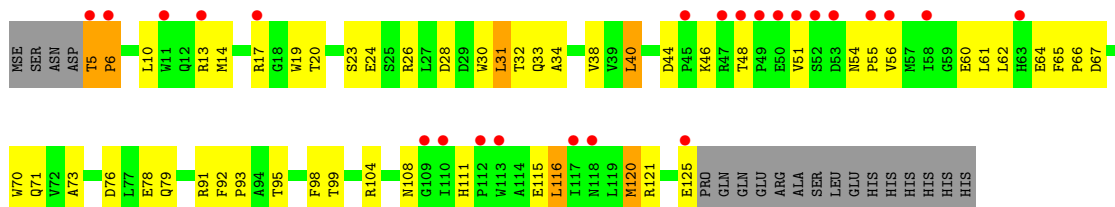
- Molecule 1: Hydrogenase-1 operon protein hyaE



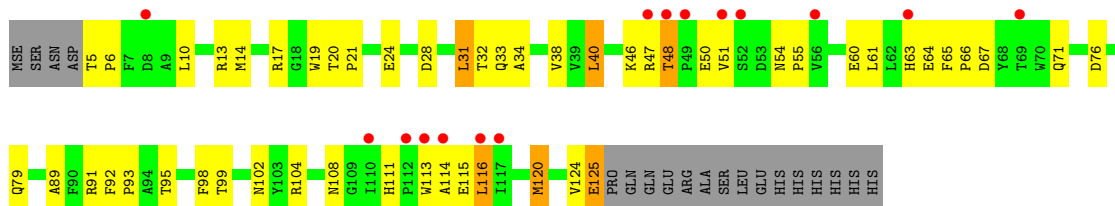
- Molecule 1: Hydrogenase-1 operon protein hyaE



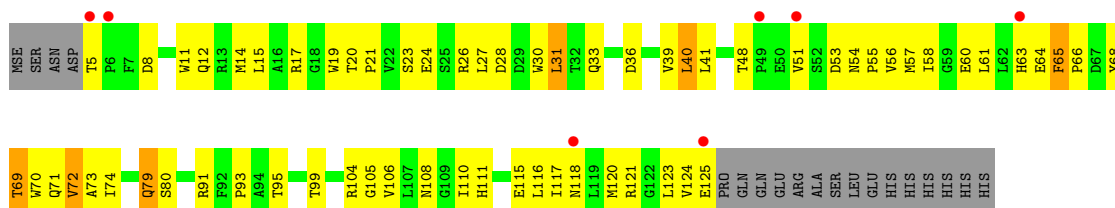
- Molecule 1: Hydrogenase-1 operon protein *hyaE*



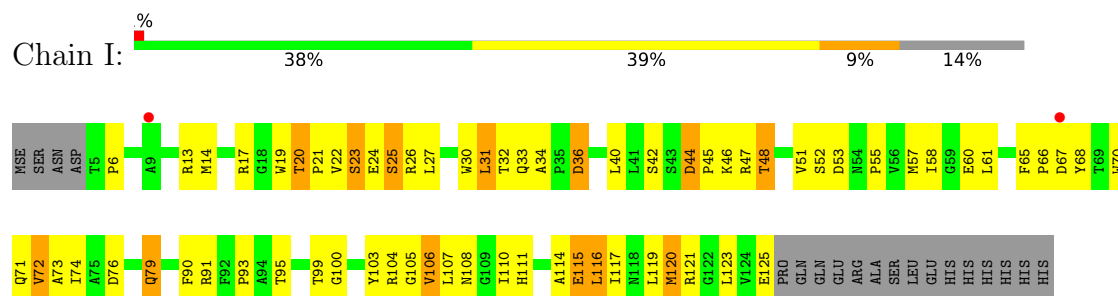
- Molecule 1: Hydrogenase-1 operon protein hyaE



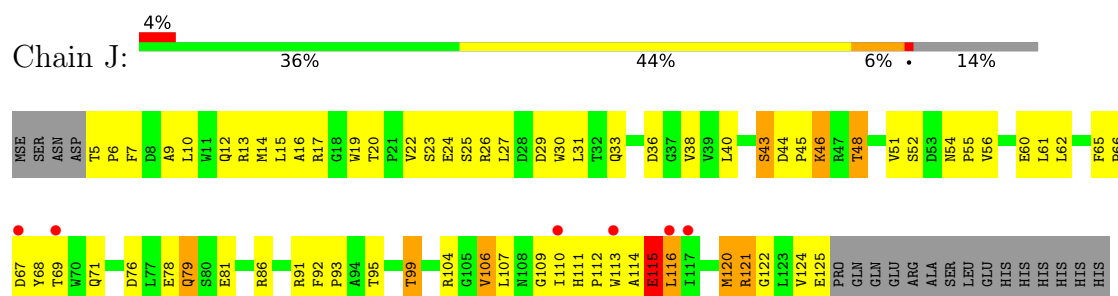
- Molecule 1: Hydrogenase-1 operon protein *hyaE*



● Molecule 1: Hydrogenase-1 operon protein hyaE



● Molecule 1: Hydrogenase-1 operon protein hyaE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.17Å 215.78Å 64.07Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	48.99 – 2.70 48.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	78.0 (48.99-2.70) 86.4 (48.99-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.41 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.292 0.272 , 0.267	Depositor DCC
R_{free} test set	7118 reflections (8.78%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9610	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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

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	0.54	0/986	0.88	2/1343 (0.1%)
1	B	0.53	0/986	0.89	2/1343 (0.1%)
1	C	0.55	0/986	0.87	3/1343 (0.2%)
1	D	0.53	0/986	0.88	2/1343 (0.1%)
1	E	0.53	0/986	0.87	1/1343 (0.1%)
1	F	0.54	0/986	0.88	3/1343 (0.2%)
1	G	0.51	0/986	0.87	0/1343
1	H	0.67	0/986	1.04	6/1343 (0.4%)
1	I	0.64	0/986	1.08	5/1343 (0.4%)
1	J	0.65	0/986	1.06	1/1343 (0.1%)
All	All	0.57	0/9860	0.94	25/13430 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	44	ASP	CA-C-N	9.87	129.49	119.82
1	I	44	ASP	C-N-CA	9.87	129.49	119.82
1	H	20	THR	N-CA-C	6.71	118.57	109.24
1	H	20	THR	CA-C-N	6.62	126.65	119.90
1	H	20	THR	C-N-CA	6.62	126.65	119.90
1	I	72	VAL	N-CA-C	5.97	116.71	107.99
1	H	72	VAL	N-CA-C	5.97	117.18	108.58
1	I	106	VAL	N-CA-C	5.95	116.86	108.17
1	I	20	THR	N-CA-C	5.67	117.83	109.62
1	H	65	PHE	CA-C-N	5.52	126.74	119.84
1	H	65	PHE	C-N-CA	5.52	126.74	119.84
1	B	62	LEU	N-CA-C	5.38	116.83	111.07
1	C	62	LEU	N-CA-C	5.28	116.72	111.07
1	D	62	LEU	N-CA-C	5.26	116.69	111.07
1	J	106	VAL	N-CA-C	5.15	120.06	109.34
1	F	70	TRP	N-CA-C	5.14	117.50	110.24
1	B	70	TRP	N-CA-C	5.14	117.48	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	TRP	N-CA-C	5.10	117.43	110.24
1	A	72	VAL	N-CA-C	5.10	115.31	108.17
1	F	20	THR	N-CA-C	5.09	117.00	109.62
1	F	62	LEU	N-CA-C	5.08	116.51	111.07
1	A	70	TRP	N-CA-C	5.07	117.38	110.24
1	C	20	THR	N-CA-C	5.03	116.91	109.62
1	C	70	TRP	N-CA-C	5.02	117.32	110.24
1	E	62	LEU	N-CA-C	5.01	116.43	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	961	0	926	65	0
1	B	961	0	926	57	1
1	C	961	0	926	40	0
1	D	961	0	926	49	0
1	E	961	0	926	47	0
1	F	961	0	926	47	0
1	G	961	0	926	62	1
1	H	961	0	926	64	0
1	I	961	0	926	62	0
1	J	961	0	926	81	0
All	All	9610	0	9260	523	1

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 28.

All (523) 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:I:14:MSE:HE3	1:I:55:PRO:HG3	1.26	1.09
1:H:14:MSE:HE2	1:H:40:LEU:HD23	1.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:MSE:HE3	1:H:55:PRO:HB3	1.42	0.99
1:H:61:LEU:HD21	1:H:120:MSE:HG3	1.42	0.98
1:A:113:TRP:CE2	1:B:13:ARG:HG2	1.99	0.97
1:J:14:MSE:HE3	1:J:55:PRO:HG3	1.45	0.97
1:A:24:GLU:H	1:A:79:GLN:HE21	1.14	0.96
1:H:99:THR:HB	1:H:104:ARG:HE	1.31	0.96
1:E:24:GLU:H	1:E:79:GLN:HE21	1.15	0.94
1:A:113:TRP:CZ2	1:B:13:ARG:HG2	2.02	0.93
1:H:91:ARG:HD3	1:H:108:ASN:HD22	1.34	0.93
1:F:14:MSE:HE2	1:F:40:LEU:HD23	1.51	0.93
1:G:24:GLU:H	1:G:79:GLN:HE21	1.14	0.92
1:H:14:MSE:CE	1:H:40:LEU:HD23	2.00	0.92
1:C:14:MSE:HE2	1:C:40:LEU:HD23	1.52	0.91
1:B:24:GLU:H	1:B:79:GLN:HE21	1.11	0.91
1:C:24:GLU:H	1:C:79:GLN:HE21	1.14	0.91
1:E:14:MSE:HE2	1:E:40:LEU:HD23	1.53	0.90
1:A:14:MSE:HE2	1:A:40:LEU:HD23	1.54	0.90
1:D:14:MSE:HE2	1:D:40:LEU:HD23	1.51	0.90
1:B:14:MSE:HE2	1:B:40:LEU:HD23	1.51	0.89
1:F:24:GLU:H	1:F:79:GLN:HE21	1.15	0.89
1:I:36:ASP:OD2	1:I:68:TYR:HB3	1.74	0.88
1:I:99:THR:HB	1:I:104:ARG:HE	1.37	0.88
1:G:14:MSE:HE2	1:G:40:LEU:HD23	1.54	0.88
1:D:24:GLU:H	1:D:79:GLN:HE21	1.14	0.88
1:A:64:GLU:CD	1:B:13:ARG:HH12	1.84	0.85
1:I:44:ASP:OD1	1:I:46:LYS:HD3	1.77	0.85
1:I:91:ARG:HG2	1:I:108:ASN:HD22	1.42	0.85
1:A:114:ALA:HB2	1:B:16:ALA:HB1	1.58	0.84
1:A:104:ARG:NH1	1:G:102:ASN:HD21	1.75	0.84
1:J:17:ARG:HG3	1:J:17:ARG:HH11	1.42	0.83
1:B:24:GLU:H	1:B:79:GLN:NE2	1.75	0.83
1:G:24:GLU:H	1:G:79:GLN:NE2	1.77	0.82
1:B:14:MSE:CE	1:B:40:LEU:HD23	2.10	0.81
1:C:24:GLU:H	1:C:79:GLN:NE2	1.78	0.81
1:J:111:HIS:HB3	1:J:115:GLU:HB3	1.63	0.80
1:A:63:HIS:NE2	1:B:13:ARG:NH2	2.29	0.80
1:J:33:GLN:HE22	1:J:71:GLN:HE22	1.29	0.80
1:E:24:GLU:H	1:E:79:GLN:NE2	1.79	0.79
1:D:24:GLU:H	1:D:79:GLN:NE2	1.80	0.79
1:F:24:GLU:H	1:F:79:GLN:NE2	1.79	0.79
1:A:24:GLU:H	1:A:79:GLN:NE2	1.79	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:GLU:HG3	1:J:9:ALA:HB1	1.64	0.78
1:G:5:THR:HB	1:G:6:PRO:HD2	1.62	0.78
1:J:14:MSE:HE2	1:J:19:TRP:HZ3	1.50	0.77
1:G:14:MSE:CE	1:G:40:LEU:HD23	2.15	0.77
1:I:14:MSE:CE	1:I:55:PRO:HG3	2.13	0.77
1:J:121:ARG:HB2	1:J:121:ARG:NH2	2.00	0.77
1:A:113:TRP:CE2	1:B:13:ARG:CG	2.69	0.76
1:F:14:MSE:CE	1:F:40:LEU:HD23	2.15	0.76
1:D:14:MSE:CE	1:D:40:LEU:HD23	2.16	0.76
1:G:91:ARG:HH11	1:H:21:PRO:HB3	1.50	0.76
1:E:14:MSE:CE	1:E:40:LEU:HD23	2.16	0.75
1:I:13:ARG:HH11	1:I:13:ARG:HG2	1.52	0.75
1:F:99:THR:HB	1:F:104:ARG:HE	1.52	0.75
1:F:6:PRO:HG3	1:F:46:LYS:HG3	1.69	0.75
1:G:6:PRO:HG3	1:G:46:LYS:HG3	1.70	0.74
1:A:14:MSE:HE3	1:A:55:PRO:HG3	1.68	0.74
1:G:113:TRP:CE2	1:J:13:ARG:HG2	2.23	0.74
1:B:99:THR:HB	1:B:104:ARG:HE	1.53	0.74
1:A:14:MSE:CE	1:A:40:LEU:HD23	2.17	0.74
1:B:14:MSE:HE3	1:B:55:PRO:HG3	1.70	0.73
1:J:13:ARG:HG2	1:J:13:ARG:HH11	1.52	0.73
1:C:14:MSE:CE	1:C:40:LEU:HD23	2.17	0.73
1:G:113:TRP:CZ2	1:J:13:ARG:HG2	2.23	0.73
1:A:91:ARG:NH2	1:F:76:ASP:OD1	2.20	0.73
1:B:91:ARG:HG2	1:B:108:ASN:HD22	1.53	0.73
1:D:6:PRO:HG3	1:D:46:LYS:HG3	1.71	0.73
1:C:99:THR:HB	1:C:104:ARG:HE	1.54	0.72
1:A:54:ASN:HB3	1:A:55:PRO:HD3	1.72	0.72
1:C:6:PRO:HG3	1:C:46:LYS:HG3	1.72	0.72
1:G:14:MSE:HE3	1:G:55:PRO:HG3	1.70	0.72
1:G:60:GLU:HB3	1:J:13:ARG:HD2	1.71	0.72
1:A:91:ARG:HG2	1:A:108:ASN:HD22	1.54	0.72
1:B:6:PRO:HG3	1:B:46:LYS:HG3	1.70	0.72
1:E:6:PRO:HG3	1:E:46:LYS:HG3	1.71	0.72
1:G:91:ARG:NH1	1:H:21:PRO:HB3	2.05	0.72
1:H:61:LEU:HD21	1:H:120:MSE:CG	2.19	0.72
1:E:99:THR:HB	1:E:104:ARG:HE	1.55	0.71
1:G:63:HIS:NE2	1:J:13:ARG:NH2	2.37	0.71
1:I:51:VAL:HA	1:I:93:PRO:HG3	1.73	0.71
1:B:54:ASN:HB3	1:B:55:PRO:HD3	1.72	0.71
1:D:54:ASN:HB3	1:D:55:PRO:HD3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:MSE:HE3	1:F:55:PRO:HG3	1.71	0.71
1:G:54:ASN:HB3	1:G:55:PRO:HD3	1.72	0.71
1:A:6:PRO:HG3	1:A:46:LYS:HG3	1.71	0.70
1:G:91:ARG:HG2	1:G:108:ASN:HD22	1.56	0.70
1:G:99:THR:HB	1:G:104:ARG:HE	1.55	0.70
1:C:91:ARG:HG2	1:C:108:ASN:HD22	1.56	0.70
1:H:91:ARG:HH11	1:H:108:ASN:ND2	1.90	0.70
1:E:54:ASN:HB3	1:E:55:PRO:HD3	1.71	0.70
1:A:104:ARG:NH1	1:G:102:ASN:ND2	2.40	0.69
1:D:91:ARG:HG2	1:D:108:ASN:HD22	1.56	0.69
1:F:54:ASN:HB3	1:F:55:PRO:HD3	1.74	0.69
1:E:91:ARG:HG2	1:E:108:ASN:HD22	1.58	0.69
1:F:91:ARG:HG2	1:F:108:ASN:HD22	1.57	0.69
1:C:54:ASN:HB3	1:C:55:PRO:HD3	1.73	0.69
1:A:99:THR:HB	1:A:104:ARG:HE	1.58	0.69
1:D:99:THR:HB	1:D:104:ARG:HE	1.58	0.69
1:C:14:MSE:HE3	1:C:55:PRO:HG3	1.74	0.68
1:H:5:THR:HB	1:H:8:ASP:CG	2.18	0.68
1:D:14:MSE:HE3	1:D:55:PRO:HG3	1.74	0.68
1:H:91:ARG:CD	1:H:108:ASN:HD22	2.06	0.67
1:E:14:MSE:HE3	1:E:55:PRO:HG3	1.76	0.67
1:G:47:ARG:NH1	1:H:24:GLU:OE2	2.27	0.67
1:I:14:MSE:HE3	1:I:55:PRO:CG	2.16	0.67
1:E:113:TRP:HB2	1:F:60:GLU:OE2	1.94	0.67
1:B:24:GLU:N	1:B:79:GLN:HE21	1.89	0.67
1:D:89:ALA:O	1:E:26:ARG:NH2	2.28	0.66
1:J:51:VAL:HG22	1:J:93:PRO:HG3	1.77	0.66
1:H:54:ASN:HB3	1:H:55:PRO:HD3	1.77	0.66
1:I:17:ARG:HD3	1:I:19:TRP:CZ2	2.31	0.66
1:J:95:THR:O	1:J:106:VAL:HG23	1.96	0.66
1:A:104:ARG:HH11	1:G:102:ASN:HD21	1.43	0.66
1:H:23:SER:HA	1:H:79:GLN:CG	2.26	0.65
1:I:25:SER:O	1:I:26:ARG:HG2	1.96	0.65
1:J:91:ARG:NH1	1:J:109:GLY:HA2	2.12	0.65
1:J:17:ARG:HG3	1:J:17:ARG:NH1	2.11	0.65
1:C:24:GLU:N	1:C:79:GLN:HE21	1.93	0.64
1:J:13:ARG:HH11	1:J:13:ARG:CG	2.10	0.64
1:E:24:GLU:N	1:E:79:GLN:HE21	1.94	0.64
1:J:5:THR:HB	1:J:6:PRO:HD2	1.78	0.64
1:J:120:MSE:O	1:J:124:VAL:HG22	1.96	0.64
1:A:63:HIS:CE1	1:B:52:SER:HB3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:GLU:N	1:D:79:GLN:HE21	1.94	0.63
1:G:24:GLU:N	1:G:79:GLN:HE21	1.92	0.63
1:H:65:PHE:HE2	1:H:121:ARG:HD3	1.63	0.63
1:F:10:LEU:HD11	1:F:55:PRO:HG2	1.81	0.63
1:B:10:LEU:HD11	1:B:55:PRO:HG2	1.79	0.63
1:I:51:VAL:HA	1:I:93:PRO:CG	2.30	0.62
1:I:14:MSE:HE2	1:I:40:LEU:CD2	2.29	0.62
1:I:14:MSE:HE2	1:I:40:LEU:HD22	1.81	0.62
1:A:10:LEU:HD11	1:A:55:PRO:HG2	1.82	0.62
1:F:24:GLU:N	1:F:79:GLN:HE21	1.93	0.62
1:E:61:LEU:HD21	1:E:120:MSE:HG3	1.82	0.62
1:J:56:VAL:O	1:J:60:GLU:HG2	1.99	0.62
1:J:121:ARG:HB2	1:J:121:ARG:HH21	1.64	0.61
1:A:60:GLU:HG3	1:B:9:ALA:HB1	1.82	0.61
1:A:24:GLU:N	1:A:79:GLN:HE21	1.93	0.61
1:B:33:GLN:HE22	1:B:71:GLN:HE22	1.48	0.61
1:J:99:THR:HG22	1:J:104:ARG:CG	2.30	0.61
1:J:111:HIS:CB	1:J:115:GLU:HB3	2.31	0.61
1:H:23:SER:HA	1:H:79:GLN:HG3	1.82	0.61
1:D:13:ARG:HH11	1:D:13:ARG:HG2	1.66	0.60
1:G:114:ALA:HB2	1:J:16:ALA:HB1	1.83	0.60
1:H:17:ARG:NH2	1:H:56:VAL:HG22	2.17	0.60
1:H:64:GLU:CD	1:H:117:ILE:HD11	2.26	0.60
1:A:113:TRP:CZ2	1:B:13:ARG:NH1	2.67	0.60
1:G:10:LEU:HD11	1:G:55:PRO:HG2	1.82	0.60
1:J:10:LEU:HA	1:J:13:ARG:HD3	1.83	0.60
1:A:14:MSE:HE3	1:A:55:PRO:CG	2.32	0.59
1:A:13:ARG:HG2	1:A:13:ARG:HH11	1.67	0.59
1:A:113:TRP:CH2	1:B:13:ARG:NH1	2.71	0.59
1:A:33:GLN:HE22	1:A:71:GLN:HE22	1.51	0.59
1:C:10:LEU:HD11	1:C:55:PRO:HG2	1.84	0.59
1:E:13:ARG:HG2	1:E:13:ARG:HH11	1.67	0.59
1:I:58:ILE:HD11	1:I:95:THR:OG1	2.02	0.59
1:J:36:ASP:OD1	1:J:68:TYR:HB3	2.02	0.59
1:G:14:MSE:HE3	1:G:55:PRO:CG	2.33	0.59
1:B:61:LEU:HD21	1:B:120:MSE:HG3	1.84	0.59
1:D:51:VAL:HG22	1:D:93:PRO:HG3	1.84	0.59
1:I:27:LEU:HG	1:I:31:LEU:HD22	1.85	0.59
1:F:61:LEU:HD21	1:F:120:MSE:HG3	1.85	0.59
1:I:104:ARG:O	1:I:123:LEU:HD22	2.01	0.59
1:J:30:TRP:O	1:J:33:GLN:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:LEU:HD11	1:D:55:PRO:HG2	1.84	0.58
1:F:13:ARG:HG2	1:F:13:ARG:HH11	1.67	0.58
1:H:24:GLU:H	1:H:79:GLN:HG3	1.68	0.58
1:C:13:ARG:HG2	1:C:13:ARG:HH11	1.67	0.58
1:D:61:LEU:HD21	1:D:120:MSE:HG3	1.86	0.58
1:F:14:MSE:HE3	1:F:55:PRO:CG	2.33	0.58
1:H:63:HIS:C	1:H:63:HIS:CD2	2.82	0.58
1:A:92:PHE:CD1	1:F:26:ARG:HD2	2.38	0.58
1:G:89:ALA:O	1:H:26:ARG:NH2	2.36	0.58
1:H:39:VAL:HG22	1:H:73:ALA:HB3	1.85	0.58
1:C:14:MSE:HE3	1:C:55:PRO:CG	2.34	0.58
1:C:61:LEU:HD21	1:C:120:MSE:HG3	1.86	0.58
1:E:17:ARG:HD2	1:E:19:TRP:CZ2	2.39	0.58
1:H:61:LEU:HD22	1:H:116:LEU:HD21	1.85	0.58
1:A:61:LEU:HD21	1:A:120:MSE:HG3	1.85	0.57
1:A:104:ARG:HH12	1:G:102:ASN:ND2	2.01	0.57
1:I:121:ARG:O	1:I:125:GLU:HB2	2.04	0.57
1:J:14:MSE:CE	1:J:55:PRO:HG3	2.25	0.57
1:C:61:LEU:O	1:C:64:GLU:HB2	2.04	0.57
1:A:63:HIS:HB2	1:B:53:ASP:OD2	2.04	0.57
1:D:14:MSE:HE3	1:D:55:PRO:CG	2.35	0.57
1:D:28:ASP:O	1:D:32:THR:HG23	2.04	0.57
1:G:13:ARG:HG2	1:G:13:ARG:HH11	1.68	0.57
1:G:51:VAL:HG22	1:G:93:PRO:HG3	1.87	0.57
1:E:10:LEU:HD11	1:E:55:PRO:HG2	1.86	0.57
1:E:51:VAL:HG22	1:E:93:PRO:HG3	1.86	0.57
1:G:64:GLU:CD	1:J:13:ARG:HH12	2.12	0.57
1:C:51:VAL:HG22	1:C:93:PRO:HG3	1.85	0.56
1:B:13:ARG:HG2	1:B:13:ARG:HH11	1.70	0.56
1:D:17:ARG:HD2	1:D:19:TRP:CZ2	2.40	0.56
1:F:17:ARG:HD2	1:F:19:TRP:CZ2	2.41	0.56
1:I:19:TRP:CD1	1:I:72:VAL:HB	2.40	0.56
1:B:5:THR:HB	1:B:6:PRO:HD2	1.87	0.56
1:G:61:LEU:O	1:G:64:GLU:HB2	2.06	0.56
1:G:61:LEU:HD21	1:G:120:MSE:HG3	1.87	0.56
1:A:92:PHE:CE1	1:F:26:ARG:HD2	2.40	0.56
1:B:28:ASP:O	1:B:32:THR:HG23	2.06	0.56
1:G:33:GLN:HE22	1:G:71:GLN:HE22	1.52	0.56
1:A:64:GLU:OE2	1:B:56:VAL:HG22	2.06	0.56
1:B:61:LEU:HD22	1:B:116:LEU:HD22	1.87	0.56
1:D:61:LEU:HD22	1:D:116:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:GLU:OE1	1:H:117:ILE:HD11	2.06	0.55
1:E:33:GLN:HE22	1:E:71:GLN:HE22	1.52	0.55
1:H:61:LEU:O	1:H:64:GLU:HB2	2.07	0.55
1:G:28:ASP:O	1:G:32:THR:HG23	2.07	0.55
1:G:61:LEU:HD22	1:G:116:LEU:HD22	1.89	0.55
1:G:125:GLU:HA	1:G:125:GLU:OE1	2.05	0.55
1:F:28:ASP:O	1:F:32:THR:HG23	2.07	0.55
1:H:19:TRP:CD2	1:H:72:VAL:HG11	2.42	0.55
1:A:28:ASP:O	1:A:32:THR:HG23	2.06	0.55
1:B:61:LEU:O	1:B:64:GLU:HB2	2.07	0.55
1:C:61:LEU:HD22	1:C:116:LEU:HD22	1.89	0.55
1:C:28:ASP:O	1:C:32:THR:HG23	2.06	0.54
1:G:91:ARG:HH11	1:H:21:PRO:CB	2.20	0.54
1:C:33:GLN:HE22	1:C:71:GLN:HE22	1.52	0.54
1:G:17:ARG:HD2	1:G:19:TRP:CZ2	2.42	0.54
1:J:27:LEU:O	1:J:27:LEU:HD12	2.07	0.54
1:J:112:PRO:HD2	1:J:115:GLU:HB2	1.89	0.54
1:A:61:LEU:HD22	1:A:116:LEU:HD22	1.90	0.54
1:D:61:LEU:O	1:D:64:GLU:HB2	2.08	0.54
1:D:125:GLU:HA	1:D:125:GLU:OE1	2.06	0.54
1:F:33:GLN:HE22	1:F:71:GLN:HE22	1.55	0.54
1:I:90:PHE:O	1:J:22:VAL:HA	2.08	0.54
1:E:14:MSE:HE3	1:E:55:PRO:CG	2.37	0.54
1:G:63:HIS:NE2	1:J:13:ARG:CZ	2.70	0.54
1:A:17:ARG:HD2	1:A:19:TRP:CZ2	2.43	0.53
1:I:48:THR:O	1:I:51:VAL:HG23	2.07	0.53
1:A:61:LEU:O	1:A:64:GLU:HB2	2.08	0.53
1:H:61:LEU:HD13	1:H:116:LEU:HD23	1.90	0.53
1:I:23:SER:HA	1:I:79:GLN:CG	2.38	0.53
1:J:10:LEU:O	1:J:14:MSE:HG3	2.08	0.53
1:J:121:ARG:O	1:J:125:GLU:HB3	2.08	0.53
1:B:17:ARG:HD2	1:B:19:TRP:CZ2	2.44	0.53
1:F:61:LEU:O	1:F:64:GLU:HB2	2.08	0.53
1:J:99:THR:CG2	1:J:104:ARG:HE	2.21	0.53
1:E:61:LEU:O	1:E:64:GLU:HB2	2.08	0.53
1:F:61:LEU:HD22	1:F:116:LEU:HD22	1.91	0.53
1:I:23:SER:HA	1:I:79:GLN:HG2	1.90	0.53
1:B:14:MSE:HE3	1:B:55:PRO:CG	2.37	0.53
1:H:23:SER:HA	1:H:79:GLN:HG2	1.91	0.53
1:J:65:PHE:N	1:J:66:PRO:HD3	2.22	0.53
1:J:23:SER:HA	1:J:79:GLN:CG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:GLN:HE22	1:D:71:GLN:HE22	1.57	0.52
1:B:51:VAL:HG22	1:B:93:PRO:HG3	1.89	0.52
1:I:24:GLU:H	1:I:79:GLN:HE21	1.57	0.52
1:I:22:VAL:HG12	1:I:74:ILE:O	2.10	0.52
1:I:13:ARG:HG2	1:I:13:ARG:NH1	2.23	0.52
1:J:12:GLN:NE2	1:J:15:LEU:HD12	2.25	0.52
1:J:36:ASP:CG	1:J:68:TYR:HB3	2.34	0.52
1:E:28:ASP:O	1:E:32:THR:HG23	2.08	0.52
1:F:51:VAL:HG22	1:F:93:PRO:HG3	1.91	0.52
1:J:13:ARG:CG	1:J:13:ARG:NH1	2.72	0.52
1:J:36:ASP:OD1	1:J:69:THR:HG22	2.10	0.52
1:J:22:VAL:HG22	1:J:23:SER:N	2.25	0.52
1:I:40:LEU:N	1:I:40:LEU:HD12	2.25	0.51
1:J:33:GLN:HE22	1:J:71:GLN:NE2	2.03	0.51
1:C:17:ARG:HD2	1:C:19:TRP:CZ2	2.46	0.51
1:C:91:ARG:NH1	1:C:108:ASN:HD22	2.08	0.51
1:E:61:LEU:HD22	1:E:116:LEU:HD22	1.92	0.51
1:I:114:ALA:O	1:I:117:ILE:HG22	2.11	0.51
1:H:105:GLY:HA3	1:H:123:LEU:HD22	1.92	0.51
1:I:91:ARG:HG2	1:I:108:ASN:ND2	2.18	0.51
1:J:7:PHE:HZ	1:J:76:ASP:HA	1.75	0.51
1:A:63:HIS:NE2	1:B:52:SER:HB3	2.26	0.50
1:J:38:VAL:HG21	1:J:62:LEU:HD21	1.93	0.50
1:A:51:VAL:HG22	1:A:93:PRO:HG3	1.92	0.50
1:B:14:MSE:HE2	1:B:19:TRP:HZ3	1.76	0.50
1:B:33:GLN:HE22	1:B:71:GLN:NE2	2.08	0.50
1:A:64:GLU:OE2	1:B:13:ARG:NH1	2.41	0.50
1:H:17:ARG:HD2	1:H:19:TRP:CZ2	2.47	0.50
1:D:33:GLN:NE2	1:D:34:ALA:HB2	2.27	0.49
1:G:14:MSE:HE2	1:G:19:TRP:HZ3	1.77	0.49
1:I:57:MSE:HE3	1:I:116:LEU:HG	1.93	0.49
1:A:60:GLU:HB3	1:B:13:ARG:HD2	1.95	0.49
1:F:121:ARG:O	1:F:125:GLU:HB3	2.11	0.49
1:H:27:LEU:HD11	1:H:39:VAL:HG21	1.93	0.49
1:H:41:LEU:HD22	1:H:80:SER:HA	1.94	0.49
1:J:43:SER:O	1:J:44:ASP:C	2.55	0.49
1:C:5:THR:HB	1:C:6:PRO:HD2	1.95	0.49
1:H:27:LEU:HG	1:H:31:LEU:HD22	1.94	0.49
1:J:92:PHE:HA	1:J:93:PRO:C	2.37	0.49
1:D:124:VAL:O	1:D:125:GLU:HB2	2.12	0.49
1:H:30:TRP:CH2	1:H:73:ALA:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ARG:NH1	1:E:108:ASN:HD22	2.10	0.49
1:H:91:ARG:HH11	1:H:108:ASN:HD22	1.59	0.49
1:I:52:SER:O	1:I:55:PRO:HD2	2.12	0.49
1:A:60:GLU:HG3	1:B:9:ALA:CB	2.42	0.49
1:G:60:GLU:HG3	1:J:9:ALA:CB	2.39	0.49
1:G:114:ALA:HB2	1:J:16:ALA:CB	2.43	0.49
1:J:45:PRO:HA	1:J:48:THR:O	2.13	0.49
1:H:54:ASN:ND2	1:H:93:PRO:HB3	2.28	0.49
1:J:91:ARG:HH12	1:J:109:GLY:HA2	1.77	0.49
1:C:33:GLN:NE2	1:C:34:ALA:HB2	2.28	0.48
1:I:115:GLU:O	1:I:119:LEU:HG	2.13	0.48
1:J:114:ALA:C	1:J:116:LEU:H	2.21	0.48
1:A:31:LEU:HD21	1:A:98:PHE:CE2	2.49	0.48
1:B:20:THR:HA	1:B:21:PRO:HD3	1.80	0.48
1:E:31:LEU:HD21	1:E:98:PHE:CE2	2.48	0.48
1:G:33:GLN:HE22	1:G:71:GLN:NE2	2.12	0.48
1:G:113:TRP:CZ2	1:J:13:ARG:NH1	2.81	0.48
1:B:33:GLN:NE2	1:B:34:ALA:HB2	2.29	0.48
1:E:33:GLN:NE2	1:E:34:ALA:HB2	2.29	0.48
1:A:91:ARG:NH1	1:A:108:ASN:HD22	2.12	0.48
1:J:38:VAL:HG12	1:J:40:LEU:CD1	2.43	0.48
1:I:91:ARG:O	1:I:91:ARG:HG3	2.14	0.47
1:B:92:PHE:HA	1:B:93:PRO:C	2.40	0.47
1:D:85:ASP:OD2	1:E:26:ARG:NH1	2.45	0.47
1:D:91:ARG:NH1	1:D:108:ASN:HD22	2.13	0.47
1:G:91:ARG:NH1	1:H:11:TRP:HZ2	2.12	0.47
1:A:91:ARG:HD2	1:F:23:SER:HB3	1.95	0.47
1:E:5:THR:HB	1:E:6:PRO:HD2	1.97	0.47
1:J:65:PHE:C	1:J:67:ASP:H	2.23	0.47
1:A:38:VAL:CG1	1:A:95:THR:HG23	2.44	0.47
1:A:92:PHE:CG	1:F:26:ARG:HD2	2.50	0.47
1:B:14:MSE:HE2	1:B:19:TRP:CZ3	2.50	0.47
1:B:38:VAL:CG1	1:B:95:THR:HG23	2.45	0.47
1:C:38:VAL:CG1	1:C:95:THR:HG23	2.44	0.47
1:E:92:PHE:HA	1:E:93:PRO:C	2.39	0.47
1:J:78:GLU:O	1:J:81:GLU:HB2	2.15	0.47
1:J:99:THR:HG22	1:J:104:ARG:HG2	1.96	0.47
1:A:14:MSE:HE2	1:A:19:TRP:HZ3	1.79	0.47
1:C:33:GLN:HE22	1:C:71:GLN:NE2	2.13	0.47
1:G:91:ARG:NH1	1:G:108:ASN:HD22	2.12	0.47
1:J:51:VAL:HG22	1:J:93:PRO:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLN:HE22	1:A:71:GLN:NE2	2.12	0.47
1:F:91:ARG:NH1	1:F:108:ASN:HD22	2.13	0.47
1:I:76:ASP:C	1:I:76:ASP:OD2	2.58	0.47
1:F:61:LEU:HD21	1:F:120:MSE:CG	2.45	0.46
1:I:95:THR:O	1:I:106:VAL:HG23	2.15	0.46
1:H:51:VAL:HG22	1:H:93:PRO:HG3	1.97	0.46
1:I:6:PRO:HG2	1:I:46:LYS:HD2	1.96	0.46
1:D:31:LEU:HD21	1:D:98:PHE:CE2	2.50	0.46
1:F:14:MSE:HE2	1:F:19:TRP:HZ3	1.81	0.46
1:I:33:GLN:NE2	1:I:34:ALA:HB2	2.30	0.46
1:J:23:SER:HA	1:J:79:GLN:HG2	1.96	0.46
1:I:20:THR:HA	1:I:21:PRO:HD3	1.81	0.46
1:J:23:SER:HA	1:J:79:GLN:HG3	1.98	0.46
1:J:24:GLU:OE1	1:J:86:ARG:NH2	2.49	0.46
1:B:91:ARG:NH1	1:B:108:ASN:HD22	2.13	0.46
1:F:92:PHE:HA	1:F:93:PRO:C	2.39	0.46
1:J:48:THR:O	1:J:51:VAL:HG23	2.16	0.46
1:F:38:VAL:CG1	1:F:95:THR:HG23	2.46	0.46
1:H:14:MSE:HE3	1:H:55:PRO:CB	2.30	0.46
1:I:65:PHE:N	1:I:66:PRO:HD3	2.31	0.46
1:J:44:ASP:OD1	1:J:46:LYS:HB2	2.16	0.46
1:C:92:PHE:HA	1:C:93:PRO:C	2.41	0.46
1:G:14:MSE:HE2	1:G:19:TRP:CZ3	2.51	0.46
1:I:107:LEU:HD11	1:I:120:MSE:HG2	1.98	0.46
1:G:33:GLN:NE2	1:G:34:ALA:HB2	2.30	0.46
1:C:125:GLU:OE1	1:C:125:GLU:HA	2.16	0.45
1:D:38:VAL:CG1	1:D:95:THR:HG23	2.45	0.45
1:D:92:PHE:HA	1:D:93:PRO:C	2.41	0.45
1:I:14:MSE:CE	1:I:40:LEU:CD2	2.94	0.45
1:I:30:TRP:CZ2	1:I:73:ALA:HB2	2.52	0.45
1:B:38:VAL:HG13	1:B:95:THR:CG2	2.46	0.45
1:E:33:GLN:HE22	1:E:71:GLN:NE2	2.14	0.45
1:F:38:VAL:HG13	1:F:95:THR:CG2	2.46	0.45
1:I:99:THR:O	1:I:100:GLY:C	2.59	0.45
1:B:31:LEU:HD21	1:B:98:PHE:CE2	2.51	0.45
1:D:90:PHE:CE1	1:E:30:TRP:HA	2.51	0.45
1:H:23:SER:O	1:H:24:GLU:C	2.58	0.45
1:I:61:LEU:HD21	1:I:120:MSE:HG3	1.98	0.45
1:J:99:THR:HG22	1:J:104:ARG:NE	2.31	0.45
1:A:38:VAL:HG13	1:A:95:THR:CG2	2.47	0.45
1:J:52:SER:O	1:J:55:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HD21	1:B:120:MSE:CG	2.47	0.45
1:F:33:GLN:HE22	1:F:71:GLN:NE2	2.14	0.45
1:F:33:GLN:NE2	1:F:34:ALA:HB2	2.31	0.45
1:I:57:MSE:HE1	1:I:111:HIS:O	2.17	0.45
1:H:28:ASP:OD2	1:H:28:ASP:N	2.49	0.45
1:J:14:MSE:HE2	1:J:19:TRP:CZ3	2.41	0.45
1:I:21:PRO:HA	1:I:74:ILE:HG13	1.98	0.45
1:I:44:ASP:OD1	1:I:46:LYS:CD	2.57	0.45
1:I:53:ASP:O	1:I:57:MSE:HG2	2.16	0.45
1:J:30:TRP:CZ2	1:J:71:GLN:HB3	2.52	0.45
1:J:68:TYR:CD1	1:J:68:TYR:N	2.85	0.45
1:G:31:LEU:HD21	1:G:98:PHE:CE2	2.51	0.44
1:C:31:LEU:HD21	1:C:98:PHE:CE2	2.52	0.44
1:I:24:GLU:C	1:I:26:ARG:H	2.26	0.44
1:D:61:LEU:HD21	1:D:120:MSE:CG	2.47	0.44
1:E:13:ARG:HH11	1:E:13:ARG:CG	2.31	0.44
1:H:5:THR:HB	1:H:8:ASP:OD1	2.17	0.44
1:H:17:ARG:HH21	1:H:56:VAL:HG22	1.82	0.44
1:E:38:VAL:CG1	1:E:95:THR:HG23	2.47	0.44
1:G:92:PHE:HA	1:G:93:PRO:C	2.41	0.44
1:H:57:MSE:HE1	1:H:110:ILE:HG13	1.99	0.44
1:C:14:MSE:HE3	1:C:55:PRO:CB	2.48	0.44
1:C:44:ASP:OD1	1:C:46:LYS:HD3	2.18	0.44
1:D:38:VAL:HG13	1:D:95:THR:CG2	2.48	0.44
1:E:61:LEU:HD21	1:E:120:MSE:CG	2.46	0.44
1:H:124:VAL:O	1:H:125:GLU:HB2	2.17	0.44
1:C:91:ARG:NH1	1:C:108:ASN:ND2	2.66	0.44
1:I:47:ARG:C	1:I:48:THR:HG22	2.42	0.44
1:D:33:GLN:HE22	1:D:71:GLN:NE2	2.15	0.44
1:J:120:MSE:C	1:J:122:GLY:H	2.26	0.44
1:A:61:LEU:HD21	1:A:120:MSE:CG	2.47	0.43
1:F:5:THR:HB	1:F:6:PRO:HD2	1.99	0.43
1:H:91:ARG:HD3	1:H:108:ASN:ND2	2.17	0.43
1:I:13:ARG:NH1	1:I:13:ARG:CG	2.78	0.43
1:A:33:GLN:NE2	1:A:34:ALA:HB2	2.33	0.43
1:A:92:PHE:HA	1:A:93:PRO:C	2.43	0.43
1:C:14:MSE:HE3	1:C:55:PRO:HB3	1.99	0.43
1:C:65:PHE:N	1:C:66:PRO:HD3	2.33	0.43
1:G:13:ARG:HH11	1:G:13:ARG:CG	2.32	0.43
1:I:19:TRP:CD2	1:I:72:VAL:HG11	2.52	0.43
1:A:76:ASP:OD2	1:A:76:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ASP:OD2	1:D:68:TYR:HD2	2.00	0.43
1:G:38:VAL:CG1	1:G:95:THR:HG23	2.47	0.43
1:H:65:PHE:N	1:H:66:PRO:HD3	2.32	0.43
1:A:14:MSE:HE2	1:A:19:TRP:CZ3	2.53	0.43
1:C:38:VAL:HG13	1:C:95:THR:CG2	2.48	0.43
1:E:65:PHE:N	1:E:66:PRO:HD3	2.34	0.43
1:F:31:LEU:HD21	1:F:98:PHE:CE2	2.53	0.43
1:H:65:PHE:CE2	1:H:121:ARG:HD3	2.48	0.43
1:A:20:THR:HA	1:A:21:PRO:HD3	1.81	0.43
1:D:14:MSE:HE3	1:D:55:PRO:HB3	2.01	0.43
1:J:99:THR:HG22	1:J:104:ARG:HE	1.83	0.43
1:A:92:PHE:CZ	1:F:26:ARG:HD2	2.52	0.43
1:E:76:ASP:OD2	1:E:76:ASP:C	2.62	0.43
1:F:6:PRO:HG3	1:F:46:LYS:CG	2.43	0.43
1:F:14:MSE:HE3	1:F:55:PRO:CB	2.49	0.43
1:I:44:ASP:HA	1:I:45:PRO:HD3	1.85	0.43
1:D:20:THR:HA	1:D:21:PRO:HD3	1.82	0.43
1:H:58:ILE:HD13	1:H:95:THR:OG1	2.18	0.43
1:H:106:VAL:O	1:H:106:VAL:HG13	2.18	0.43
1:D:6:PRO:HG3	1:D:46:LYS:CG	2.45	0.42
1:F:14:MSE:HE2	1:F:19:TRP:CZ3	2.54	0.42
1:G:6:PRO:HG3	1:G:46:LYS:CG	2.44	0.42
1:A:13:ARG:HH11	1:A:13:ARG:CG	2.30	0.42
1:B:30:TRP:CZ2	1:B:73:ALA:HB2	2.54	0.42
1:B:48:THR:C	1:B:50:GLU:H	2.27	0.42
1:H:31:LEU:HD12	1:H:31:LEU:HA	1.79	0.42
1:H:99:THR:HG22	1:H:104:ARG:HH11	1.83	0.42
1:J:106:VAL:HG13	1:J:106:VAL:O	2.19	0.42
1:A:65:PHE:N	1:A:66:PRO:HD3	2.34	0.42
1:E:30:TRP:CZ2	1:E:73:ALA:HB2	2.54	0.42
1:F:14:MSE:HE3	1:F:55:PRO:HB3	2.02	0.42
1:G:20:THR:HA	1:G:21:PRO:HD3	1.80	0.42
1:G:76:ASP:OD2	1:G:76:ASP:C	2.62	0.42
1:A:91:ARG:NH1	1:A:108:ASN:ND2	2.68	0.42
1:C:19:TRP:CD1	1:C:72:VAL:HB	2.55	0.42
1:D:65:PHE:N	1:D:66:PRO:HD3	2.35	0.42
1:E:38:VAL:HG13	1:E:95:THR:CG2	2.50	0.42
1:I:6:PRO:HG2	1:I:46:LYS:CD	2.49	0.42
1:B:14:MSE:HE1	1:B:40:LEU:HD23	1.97	0.42
1:B:38:VAL:CG1	1:B:95:THR:CG2	2.98	0.42
1:C:6:PRO:HG3	1:C:46:LYS:CG	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:THR:HA	1:E:21:PRO:HD3	1.81	0.42
1:E:48:THR:C	1:E:50:GLU:H	2.27	0.42
1:F:13:ARG:HH11	1:F:13:ARG:CG	2.31	0.42
1:I:19:TRP:CG	1:I:72:VAL:HB	2.55	0.42
1:I:61:LEU:HD21	1:I:120:MSE:CG	2.49	0.42
1:A:6:PRO:HG3	1:A:46:LYS:CG	2.44	0.42
1:A:64:GLU:OE2	1:B:13:ARG:NH2	2.52	0.42
1:B:6:PRO:HG3	1:B:46:LYS:CG	2.44	0.42
1:J:10:LEU:O	1:J:13:ARG:HB2	2.20	0.42
1:C:48:THR:C	1:C:50:GLU:H	2.27	0.42
1:E:14:MSE:HE3	1:E:55:PRO:HB3	2.01	0.42
1:I:30:TRP:HE3	1:I:31:LEU:HD13	1.85	0.42
1:D:14:MSE:HE2	1:D:19:TRP:HZ3	1.85	0.42
1:H:33:GLN:HE22	1:H:71:GLN:HE22	1.68	0.42
1:G:124:VAL:O	1:G:125:GLU:HB2	2.20	0.41
1:J:91:ARG:HA	1:J:91:ARG:HD2	1.93	0.41
1:C:20:THR:HA	1:C:21:PRO:HD3	1.81	0.41
1:D:65:PHE:HB2	1:D:70:TRP:HE1	1.86	0.41
1:F:65:PHE:N	1:F:66:PRO:HD3	2.36	0.41
1:G:91:ARG:NH1	1:G:108:ASN:ND2	2.69	0.41
1:H:8:ASP:O	1:H:12:GLN:HG2	2.20	0.41
1:H:69:THR:O	1:H:69:THR:OG1	2.39	0.41
1:I:103:TYR:CE2	1:I:105:GLY:O	2.73	0.41
1:D:14:MSE:HE3	1:D:55:PRO:CB	2.50	0.41
1:E:6:PRO:HG3	1:E:46:LYS:CG	2.46	0.41
1:G:38:VAL:HG13	1:G:95:THR:CG2	2.49	0.41
1:H:36:ASP:OD2	1:H:68:TYR:HB3	2.19	0.41
1:I:66:PRO:O	1:I:67:ASP:C	2.61	0.41
1:D:90:PHE:HA	1:E:26:ARG:HD3	2.01	0.41
1:F:44:ASP:OD1	1:F:46:LYS:HD3	2.20	0.41
1:H:117:ILE:HG23	1:H:118:ASN:N	2.34	0.41
1:J:107:LEU:HD11	1:J:120:MSE:HG2	2.02	0.41
1:D:48:THR:C	1:D:50:GLU:H	2.28	0.41
1:E:30:TRP:O	1:E:33:GLN:HG3	2.21	0.41
1:C:13:ARG:HH11	1:C:13:ARG:CG	2.31	0.41
1:I:6:PRO:HD2	1:I:46:LYS:HE3	2.02	0.41
1:J:61:LEU:HD21	1:J:120:MSE:CG	2.51	0.41
1:B:65:PHE:N	1:B:66:PRO:HD3	2.36	0.41
1:D:6:PRO:HG2	1:D:7:PHE:H	1.86	0.41
1:J:48:THR:O	1:J:48:THR:HG23	2.20	0.41
1:E:91:ARG:NH1	1:E:108:ASN:ND2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:THR:C	1:G:50:GLU:H	2.29	0.41
1:G:61:LEU:HD21	1:G:120:MSE:CG	2.49	0.41
1:D:13:ARG:HH11	1:D:13:ARG:CG	2.30	0.41
1:D:64:GLU:HG3	1:D:113:TRP:CH2	2.56	0.41
1:E:14:MSE:HE3	1:E:55:PRO:CB	2.51	0.41
1:G:64:GLU:HG3	1:G:113:TRP:CH2	2.56	0.41
1:I:65:PHE:HB2	1:I:70:TRP:HE1	1.86	0.41
1:J:110:ILE:O	1:J:110:ILE:HG23	2.20	0.41
1:B:76:ASP:C	1:B:76:ASP:OD2	2.64	0.41
1:C:61:LEU:HD21	1:C:120:MSE:CG	2.49	0.41
1:J:112:PRO:O	1:J:113:TRP:C	2.63	0.41
1:G:65:PHE:N	1:G:66:PRO:HD3	2.35	0.40
1:H:27:LEU:O	1:H:31:LEU:HB2	2.21	0.40
1:H:60:GLU:O	1:H:61:LEU:C	2.64	0.40
1:I:60:GLU:O	1:I:61:LEU:C	2.64	0.40
1:D:91:ARG:NH1	1:D:108:ASN:ND2	2.69	0.40
1:D:92:PHE:CZ	1:E:26:ARG:HD2	2.57	0.40
1:H:60:GLU:OE2	1:H:63:HIS:CE1	2.74	0.40
1:H:74:ILE:HD13	1:H:74:ILE:HG21	1.86	0.40
1:J:46:LYS:HB2	1:J:46:LYS:HE2	1.90	0.40
1:B:19:TRP:CD1	1:B:72:VAL:HB	2.57	0.40
1:A:48:THR:C	1:A:50:GLU:H	2.30	0.40
1:A:115:GLU:O	1:A:118:ASN:OD1	2.40	0.40
1:D:30:TRP:O	1:D:33:GLN:HG3	2.22	0.40
1:E:36:ASP:OD2	1:E:68:TYR:HD2	2.04	0.40
1:F:30:TRP:CZ2	1:F:73:ALA:HB2	2.56	0.40
1:F:78:GLU:H	1:F:78:GLU:CD	2.30	0.40
1:H:30:TRP:CZ2	1:H:73:ALA:HB2	2.56	0.40
1:J:13:ARG:NH1	1:J:13:ARG:HB3	2.37	0.40

All (1) 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:B:91:ARG:NH2	1:G:76:ASP:OD1[1_655]	2.12	0.08

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	B	56/140 (40%)	55 (98%)	1 (2%)	0	100	100
1	C	119/140 (85%)	114 (96%)	5 (4%)	0	100	100
1	D	119/140 (85%)	115 (97%)	4 (3%)	0	100	100
1	E	119/140 (85%)	112 (94%)	7 (6%)	0	100	100
1	F	111/140 (79%)	108 (97%)	2 (2%)	1 (1%)	14	35
1	G	119/140 (85%)	114 (96%)	5 (4%)	0	100	100
1	H	119/140 (85%)	107 (90%)	11 (9%)	1 (1%)	16	37
1	I	119/140 (85%)	108 (91%)	10 (8%)	1 (1%)	16	37
1	J	111/140 (79%)	96 (86%)	14 (13%)	1 (1%)	14	35
All	All	992/1260 (79%)	929 (94%)	59 (6%)	4 (0%)	30	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	25	SER
1	J	115	GLU
1	F	6	PRO
1	H	70	TRP

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	102/116 (88%)	93 (91%)	9 (9%)	9	23
1	B	102/116 (88%)	94 (92%)	8 (8%)	11	29
1	C	102/116 (88%)	94 (92%)	8 (8%)	11	29
1	D	102/116 (88%)	93 (91%)	9 (9%)	9	23
1	E	102/116 (88%)	93 (91%)	9 (9%)	9	23
1	F	102/116 (88%)	92 (90%)	10 (10%)	7	19
1	G	102/116 (88%)	93 (91%)	9 (9%)	9	23
1	H	102/116 (88%)	93 (91%)	9 (9%)	9	23
1	I	102/116 (88%)	90 (88%)	12 (12%)	5	13
1	J	102/116 (88%)	87 (85%)	15 (15%)	3	8
All	All	1020/1160 (88%)	922 (90%)	98 (10%)	8	20

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	40	LEU
1	A	48	THR
1	A	56	VAL
1	A	67	ASP
1	A	111	HIS
1	A	115	GLU
1	A	116	LEU
1	A	120	MSE
1	B	31	LEU
1	B	40	LEU
1	B	48	THR
1	B	67	ASP
1	B	111	HIS
1	B	115	GLU
1	B	116	LEU
1	B	120	MSE
1	C	31	LEU
1	C	40	LEU
1	C	48	THR
1	C	67	ASP
1	C	111	HIS
1	C	115	GLU
1	C	116	LEU

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Mol	Chain	Res	Type
1	C	120	MSE
1	D	5	THR
1	D	31	LEU
1	D	40	LEU
1	D	48	THR
1	D	67	ASP
1	D	111	HIS
1	D	115	GLU
1	D	116	LEU
1	D	120	MSE
1	E	5	THR
1	E	31	LEU
1	E	40	LEU
1	E	48	THR
1	E	67	ASP
1	E	111	HIS
1	E	115	GLU
1	E	116	LEU
1	E	120	MSE
1	F	5	THR
1	F	31	LEU
1	F	40	LEU
1	F	48	THR
1	F	56	VAL
1	F	67	ASP
1	F	111	HIS
1	F	115	GLU
1	F	116	LEU
1	F	120	MSE
1	G	31	LEU
1	G	40	LEU
1	G	48	THR
1	G	67	ASP
1	G	111	HIS
1	G	115	GLU
1	G	116	LEU
1	G	120	MSE
1	G	125	GLU
1	H	15	LEU
1	H	31	LEU
1	H	40	LEU
1	H	48	THR

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Mol	Chain	Res	Type
1	H	53	ASP
1	H	69	THR
1	H	79	GLN
1	H	111	HIS
1	H	115	GLU
1	I	23	SER
1	I	31	LEU
1	I	32	THR
1	I	36	ASP
1	I	42	SER
1	I	48	THR
1	I	71	GLN
1	I	79	GLN
1	I	110	ILE
1	I	115	GLU
1	I	116	LEU
1	I	120	MSE
1	J	20	THR
1	J	25	SER
1	J	26	ARG
1	J	29	ASP
1	J	31	LEU
1	J	43	SER
1	J	46	LYS
1	J	48	THR
1	J	54	ASN
1	J	79	GLN
1	J	99	THR
1	J	115	GLU
1	J	116	LEU
1	J	120	MSE
1	J	121	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	79	GLN
1	A	102	ASN
1	A	108	ASN
1	B	33	GLN
1	B	71	GLN

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Mol	Chain	Res	Type
1	B	79	GLN
1	B	102	ASN
1	B	108	ASN
1	C	33	GLN
1	C	79	GLN
1	C	102	ASN
1	C	108	ASN
1	D	33	GLN
1	D	71	GLN
1	D	79	GLN
1	D	102	ASN
1	D	108	ASN
1	E	33	GLN
1	E	79	GLN
1	E	102	ASN
1	E	108	ASN
1	F	71	GLN
1	F	79	GLN
1	F	102	ASN
1	F	108	ASN
1	G	33	GLN
1	G	71	GLN
1	G	79	GLN
1	G	102	ASN
1	G	108	ASN
1	H	33	GLN
1	H	54	ASN
1	H	63	HIS
1	H	71	GLN
1	H	102	ASN
1	H	108	ASN
1	I	12	GLN
1	I	79	GLN
1	I	102	ASN
1	I	108	ASN
1	J	12	GLN
1	J	54	ASN
1	J	71	GLN
1	J	79	GLN
1	J	102	ASN
1	J	108	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	118/140 (84%)	1.17	24 (20%) 3 2	34, 59, 96, 103	0
1	B	118/140 (84%)	0.95	18 (15%) 5 4	37, 53, 90, 96	0
1	C	118/140 (84%)	0.69	15 (12%) 8 7	29, 54, 81, 89	0
1	D	118/140 (84%)	0.76	10 (8%) 16 14	35, 57, 86, 92	0
1	E	118/140 (84%)	0.87	8 (6%) 23 20	32, 57, 84, 91	0
1	F	118/140 (84%)	1.14	24 (20%) 3 2	34, 56, 92, 103	0
1	G	118/140 (84%)	0.94	15 (12%) 8 7	39, 57, 95, 97	0
1	H	118/140 (84%)	0.47	7 (5%) 28 25	33, 47, 79, 92	0
1	I	118/140 (84%)	0.35	2 (1%) 69 67	31, 51, 73, 85	0
1	J	118/140 (84%)	0.56	6 (5%) 33 29	33, 53, 83, 90	0
All	All	1180/1400 (84%)	0.79	129 (10%) 10 9	29, 54, 87, 103	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	51	VAL	9.7
1	G	113	TRP	8.3
1	A	113	TRP	7.6
1	A	51	VAL	7.4
1	F	52	SER	5.5
1	H	51	VAL	5.5
1	A	48	THR	5.3
1	F	110	ILE	5.1
1	G	51	VAL	4.8
1	A	52	SER	4.7
1	A	63	HIS	4.7
1	F	48	THR	4.5
1	G	63	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	48	THR	4.1
1	B	116	LEU	4.1
1	B	113	TRP	4.1
1	F	49	PRO	4.0
1	A	115	GLU	4.0
1	A	112	PRO	3.8
1	E	112	PRO	3.8
1	E	58	ILE	3.8
1	H	63	HIS	3.8
1	F	6	PRO	3.8
1	B	110	ILE	3.7
1	D	110	ILE	3.7
1	C	113	TRP	3.7
1	D	124	VAL	3.6
1	F	113	TRP	3.6
1	A	56	VAL	3.5
1	A	110	ILE	3.5
1	D	58	ILE	3.5
1	A	49	PRO	3.4
1	F	125	GLU	3.4
1	G	114	ALA	3.3
1	F	53	ASP	3.3
1	B	63	HIS	3.3
1	F	117	ILE	3.3
1	C	47	ARG	3.2
1	D	47	ARG	3.2
1	B	55	PRO	3.2
1	E	113	TRP	3.2
1	J	113	TRP	3.2
1	B	112	PRO	3.2
1	E	117	ILE	3.2
1	C	13	ARG	3.1
1	G	56	VAL	3.1
1	A	117	ILE	3.1
1	A	114	ALA	3.0
1	F	5	THR	3.0
1	D	113	TRP	3.0
1	B	54	ASN	3.0
1	A	53	ASP	3.0
1	F	47	ARG	3.0
1	A	119	LEU	2.9
1	A	111	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	47	ARG	2.9
1	B	48	THR	2.8
1	C	49	PRO	2.8
1	A	50	GLU	2.8
1	B	56	VAL	2.8
1	G	112	PRO	2.7
1	G	117	ILE	2.6
1	F	112	PRO	2.6
1	A	31	LEU	2.6
1	G	116	LEU	2.6
1	C	111	HIS	2.6
1	C	48	THR	2.6
1	F	50	GLU	2.6
1	C	112	PRO	2.6
1	G	49	PRO	2.6
1	E	110	ILE	2.6
1	B	60	GLU	2.6
1	H	49	PRO	2.5
1	C	110	ILE	2.5
1	G	110	ILE	2.5
1	B	50	GLU	2.5
1	C	50	GLU	2.5
1	J	69	THR	2.5
1	G	52	SER	2.5
1	J	117	ILE	2.5
1	F	56	VAL	2.5
1	B	114	ALA	2.5
1	H	5	THR	2.4
1	J	110	ILE	2.4
1	F	17	ARG	2.4
1	H	118	ASN	2.4
1	A	55	PRO	2.4
1	H	125	GLU	2.4
1	B	51	VAL	2.4
1	H	6	PRO	2.4
1	F	58	ILE	2.3
1	A	54	ASN	2.3
1	C	125	GLU	2.3
1	E	60	GLU	2.3
1	G	8	ASP	2.3
1	D	51	VAL	2.3
1	C	58	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	69	THR	2.3
1	D	50	GLU	2.3
1	B	109	GLY	2.3
1	C	118	ASN	2.2
1	F	55	PRO	2.2
1	D	56	VAL	2.2
1	I	9	ALA	2.2
1	A	64	GLU	2.2
1	A	125	GLU	2.2
1	B	67	ASP	2.2
1	D	22	VAL	2.2
1	B	58	ILE	2.2
1	F	45	PRO	2.2
1	J	116	LEU	2.2
1	I	67	ASP	2.2
1	J	67	ASP	2.2
1	A	116	LEU	2.1
1	F	109	GLY	2.1
1	C	63	HIS	2.1
1	F	11	TRP	2.1
1	E	55	PRO	2.1
1	F	118	ASN	2.1
1	F	63	HIS	2.1
1	F	13	ARG	2.1
1	C	55	PRO	2.1
1	A	118	ASN	2.1
1	A	60	GLU	2.1
1	E	13	ARG	2.0
1	B	49	PRO	2.0
1	C	16	ALA	2.0
1	B	47	ARG	2.0
1	D	13	ARG	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.