



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:28 AM UTC

PDB ID : 8ZWD / pdb_00008zwd
Title : Crystal structure of methanol dehydrogenase1 from Bacillus methanolicus
Authors : Ma, B.D.; Kong, X.D.
Deposited on : 2024-06-12
Resolution : 3.00 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

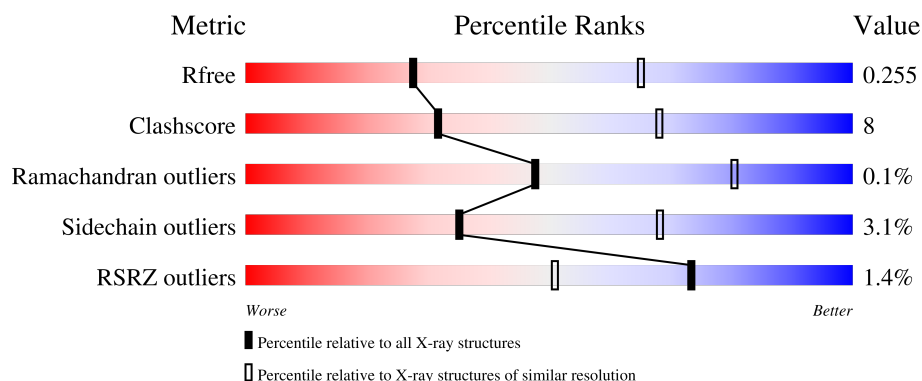
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	390	 79% 19% .
1	B	390	 81% 17% ..
1	C	390	 78% 20% ..
1	D	390	 79% 18% ..
1	E	390	 77% 20% ..

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Mol	Chain	Length	Quality of chain
1	F	390	3% 76% 21% ..
1	G	390	% 69% 17% 14%
1	H	390	2% 77% 21% ..
1	I	390	81% 15% ..
1	J	390	5% 70% 23% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27906 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 NAD(P)-dependent methanol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	384	Total	C	N	O	S	0	1	0
			2840	1787	486	553	14			
1	D	384	Total	C	N	O	S	0	0	0
			2834	1783	486	551	14			
1	H	384	Total	C	N	O	S	0	0	0
			2834	1783	486	551	14			
1	J	369	Total	C	N	O	S	0	0	0
			2721	1719	462	526	14			
1	E	384	Total	C	N	O	S	0	1	0
			2842	1788	489	551	14			
1	G	335	Total	C	N	O	S	0	0	0
			2470	1558	421	479	12			
1	F	384	Total	C	N	O	S	0	0	0
			2834	1783	486	551	14			
1	C	384	Total	C	N	O	S	0	0	0
			2834	1783	486	551	14			
1	A	384	Total	C	N	O	S	0	0	0
			2834	1783	486	551	14			
1	I	383	Total	C	N	O	S	0	0	0
			2826	1778	485	550	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	383	LEU	-	expression tag	UNP Q6TV41
B	384	GLU	-	expression tag	UNP Q6TV41
B	385	HIS	-	expression tag	UNP Q6TV41
B	386	HIS	-	expression tag	UNP Q6TV41
B	387	HIS	-	expression tag	UNP Q6TV41
B	388	HIS	-	expression tag	UNP Q6TV41
B	389	HIS	-	expression tag	UNP Q6TV41
B	390	HIS	-	expression tag	UNP Q6TV41
D	383	LEU	-	expression tag	UNP Q6TV41

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Chain	Residue	Modelled	Actual	Comment	Reference
D	384	GLU	-	expression tag	UNP Q6TV41
D	385	HIS	-	expression tag	UNP Q6TV41
D	386	HIS	-	expression tag	UNP Q6TV41
D	387	HIS	-	expression tag	UNP Q6TV41
D	388	HIS	-	expression tag	UNP Q6TV41
D	389	HIS	-	expression tag	UNP Q6TV41
D	390	HIS	-	expression tag	UNP Q6TV41
H	383	LEU	-	expression tag	UNP Q6TV41
H	384	GLU	-	expression tag	UNP Q6TV41
H	385	HIS	-	expression tag	UNP Q6TV41
H	386	HIS	-	expression tag	UNP Q6TV41
H	387	HIS	-	expression tag	UNP Q6TV41
H	388	HIS	-	expression tag	UNP Q6TV41
H	389	HIS	-	expression tag	UNP Q6TV41
H	390	HIS	-	expression tag	UNP Q6TV41
J	383	LEU	-	expression tag	UNP Q6TV41
J	384	GLU	-	expression tag	UNP Q6TV41
J	385	HIS	-	expression tag	UNP Q6TV41
J	386	HIS	-	expression tag	UNP Q6TV41
J	387	HIS	-	expression tag	UNP Q6TV41
J	388	HIS	-	expression tag	UNP Q6TV41
J	389	HIS	-	expression tag	UNP Q6TV41
J	390	HIS	-	expression tag	UNP Q6TV41
E	383	LEU	-	expression tag	UNP Q6TV41
E	384	GLU	-	expression tag	UNP Q6TV41
E	385	HIS	-	expression tag	UNP Q6TV41
E	386	HIS	-	expression tag	UNP Q6TV41
E	387	HIS	-	expression tag	UNP Q6TV41
E	388	HIS	-	expression tag	UNP Q6TV41
E	389	HIS	-	expression tag	UNP Q6TV41
E	390	HIS	-	expression tag	UNP Q6TV41
G	383	LEU	-	expression tag	UNP Q6TV41
G	384	GLU	-	expression tag	UNP Q6TV41
G	385	HIS	-	expression tag	UNP Q6TV41
G	386	HIS	-	expression tag	UNP Q6TV41
G	387	HIS	-	expression tag	UNP Q6TV41
G	388	HIS	-	expression tag	UNP Q6TV41
G	389	HIS	-	expression tag	UNP Q6TV41
G	390	HIS	-	expression tag	UNP Q6TV41
F	383	LEU	-	expression tag	UNP Q6TV41
F	384	GLU	-	expression tag	UNP Q6TV41
F	385	HIS	-	expression tag	UNP Q6TV41

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Chain	Residue	Modelled	Actual	Comment	Reference
F	386	HIS	-	expression tag	UNP Q6TV41
F	387	HIS	-	expression tag	UNP Q6TV41
F	388	HIS	-	expression tag	UNP Q6TV41
F	389	HIS	-	expression tag	UNP Q6TV41
F	390	HIS	-	expression tag	UNP Q6TV41
C	383	LEU	-	expression tag	UNP Q6TV41
C	384	GLU	-	expression tag	UNP Q6TV41
C	385	HIS	-	expression tag	UNP Q6TV41
C	386	HIS	-	expression tag	UNP Q6TV41
C	387	HIS	-	expression tag	UNP Q6TV41
C	388	HIS	-	expression tag	UNP Q6TV41
C	389	HIS	-	expression tag	UNP Q6TV41
C	390	HIS	-	expression tag	UNP Q6TV41
A	383	LEU	-	expression tag	UNP Q6TV41
A	384	GLU	-	expression tag	UNP Q6TV41
A	385	HIS	-	expression tag	UNP Q6TV41
A	386	HIS	-	expression tag	UNP Q6TV41
A	387	HIS	-	expression tag	UNP Q6TV41
A	388	HIS	-	expression tag	UNP Q6TV41
A	389	HIS	-	expression tag	UNP Q6TV41
A	390	HIS	-	expression tag	UNP Q6TV41
I	383	LEU	-	expression tag	UNP Q6TV41
I	384	GLU	-	expression tag	UNP Q6TV41
I	385	HIS	-	expression tag	UNP Q6TV41
I	386	HIS	-	expression tag	UNP Q6TV41
I	387	HIS	-	expression tag	UNP Q6TV41
I	388	HIS	-	expression tag	UNP Q6TV41
I	389	HIS	-	expression tag	UNP Q6TV41
I	390	HIS	-	expression tag	UNP Q6TV41

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0
2	J	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 1	0	0
2	I	1	Total 1	Mn 1	0	0

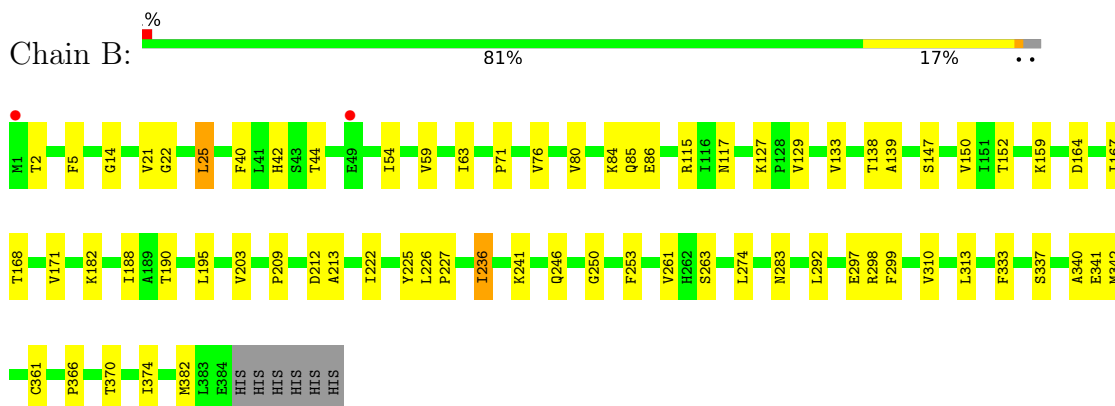
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	6	Total 6	O 6	0	0
3	D	4	Total 4	O 4	0	0
3	H	3	Total 3	O 3	0	0
3	J	2	Total 2	O 2	0	0
3	G	1	Total 1	O 1	0	0
3	F	1	Total 1	O 1	0	0
3	C	2	Total 2	O 2	0	0
3	A	6	Total 6	O 6	0	0
3	I	2	Total 2	O 2	0	0

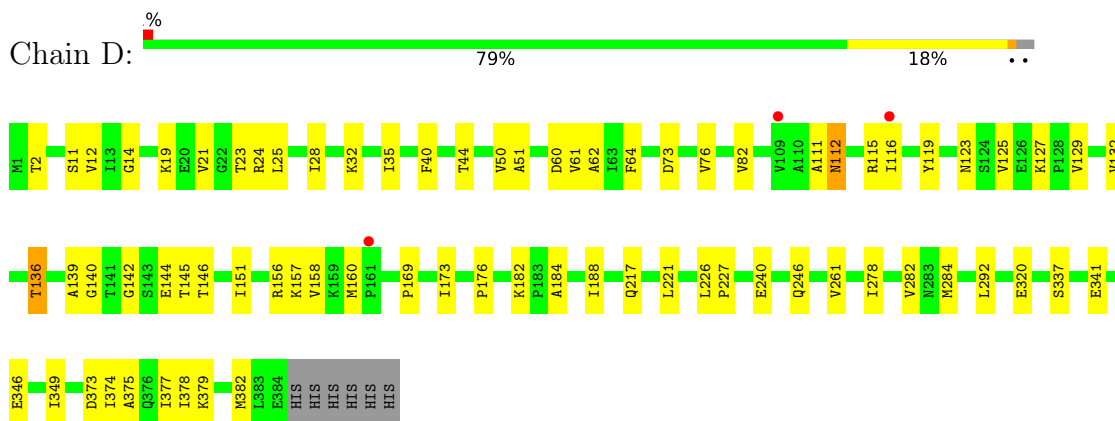
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

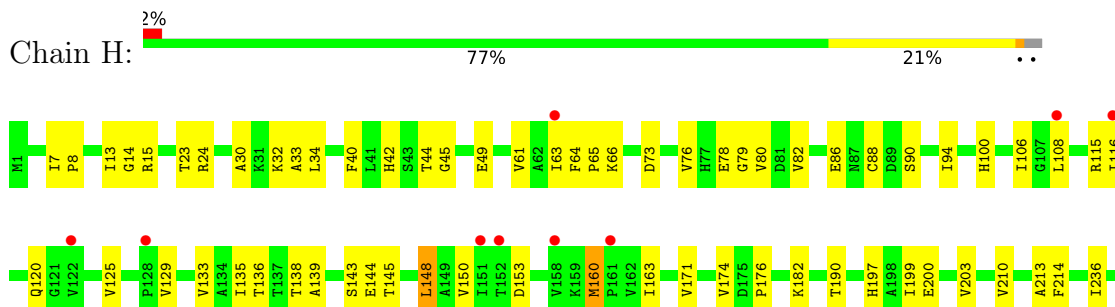
- Molecule 1: NAD(P)-dependent methanol dehydrogenase



- Molecule 1: NAD(P)-dependent methanol dehydrogenase

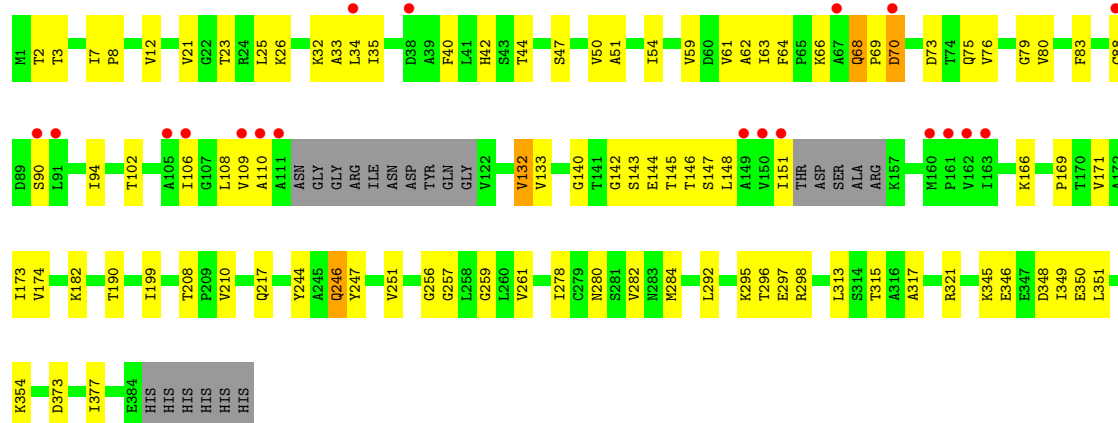


- Molecule 1: NAD(P)-dependent methanol dehydrogenase

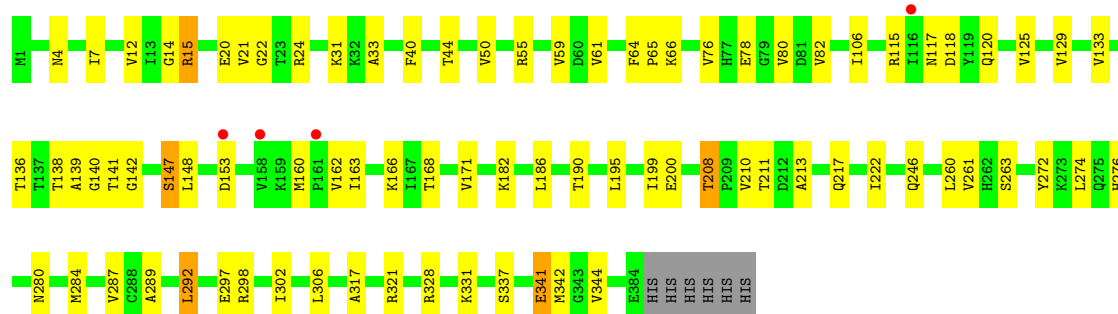
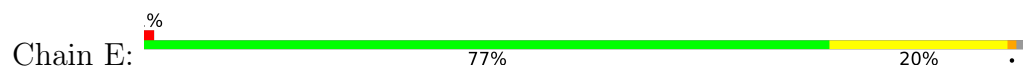




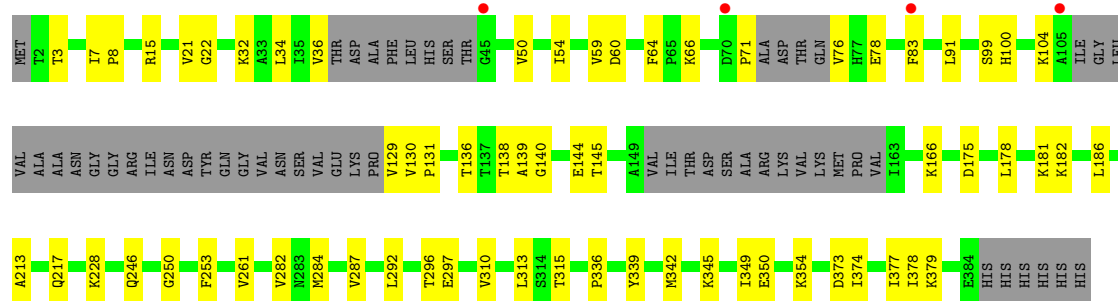
- Molecule 1: NAD(P)-dependent methanol dehydrogenase



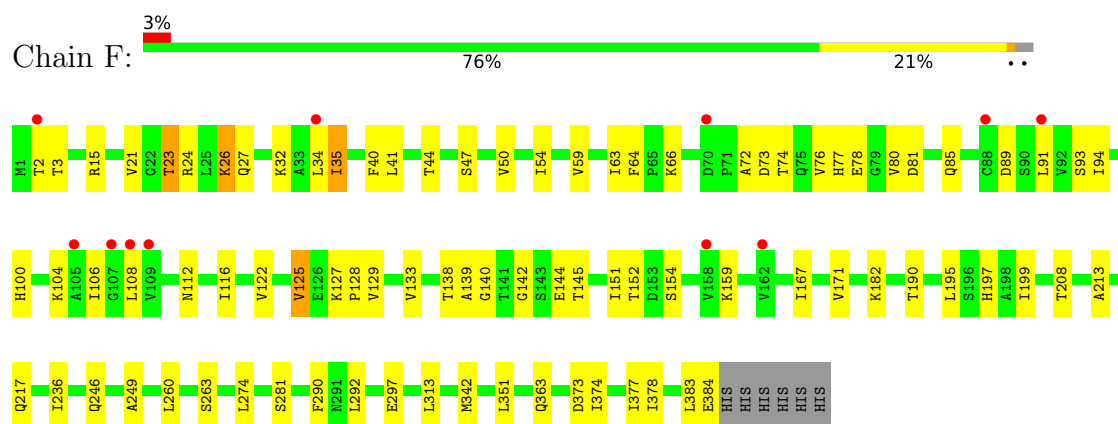
- Molecule 1: NAD(P)-dependent methanol dehydrogenase



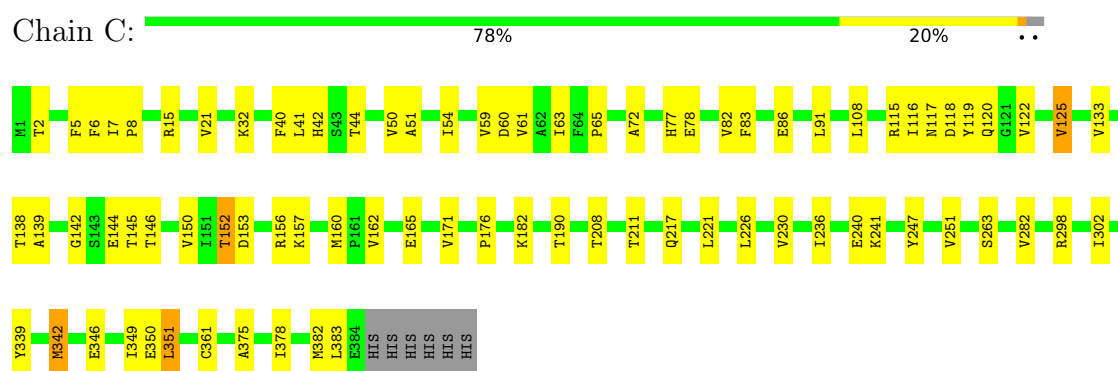
- Molecule 1: NAD(P)-dependent methanol dehydrogenase



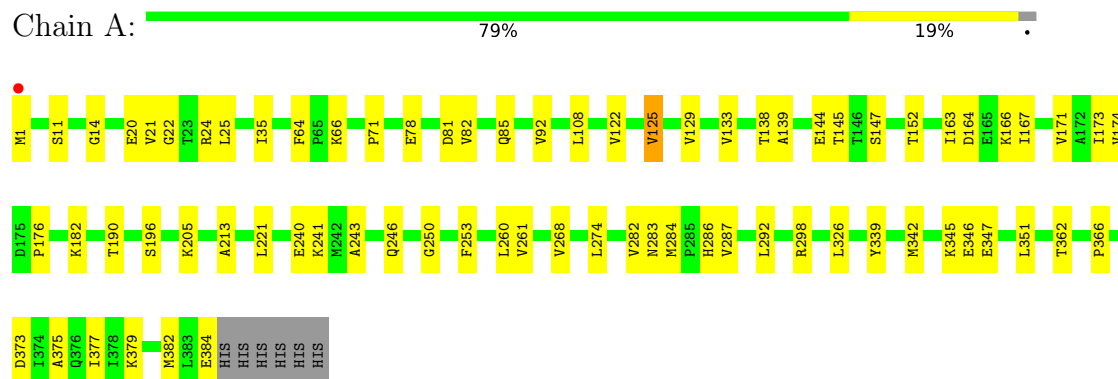
- Molecule 1: NAD(P)-dependent methanol dehydrogenase



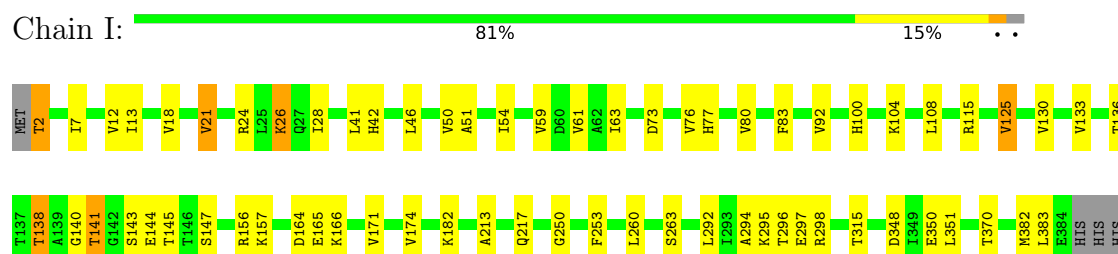
- Molecule 1: NAD(P)-dependent methanol dehydrogenase



- Molecule 1: NAD(P)-dependent methanol dehydrogenase



- Molecule 1: NAD(P)-dependent methanol dehydrogenase



HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	256.02Å 83.58Å 220.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.13 – 3.00 30.13 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.5 (30.13-3.00) 95.4 (30.13-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.214 , 0.261 0.212 , 0.255	Depositor DCC
R_{free} test set	4526 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27906	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.28	0/2877	0.45	0/3906
1	B	0.35	0/2886	0.47	0/3918
1	C	0.31	0/2877	0.45	1/3906 (0.0%)
1	D	0.35	0/2877	0.47	0/3906
1	E	0.23	0/2888	0.43	0/3920
1	F	0.40	0/2877	0.51	1/3906 (0.0%)
1	G	0.31	0/2504	0.47	1/3393 (0.0%)
1	H	0.31	0/2877	0.47	0/3906
1	I	0.43	0/2869	0.54	3/3896 (0.1%)
1	J	0.47	0/2761	0.62	8/3747 (0.2%)
All	All	0.35	0/28293	0.49	14/38404 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	108	LEU	N-CA-C	-9.38	101.02	111.14
1	J	110	ALA	N-CA-C	-8.53	92.62	110.80
1	J	69	PRO	CA-C-O	-6.82	114.11	121.27
1	J	257	GLY	N-CA-C	6.56	119.17	111.63
1	J	69	PRO	N-CA-C	-6.32	100.72	110.95
1	I	156	ARG	N-CA-C	-6.08	100.09	109.76
1	F	290	PHE	N-CA-C	-6.06	104.59	111.14
1	G	140	GLY	N-CA-C	-6.01	102.47	111.19
1	J	259	GLY	N-CA-C	5.81	118.70	110.74
1	J	261	VAL	N-CA-C	-5.52	105.34	110.53
1	J	140	GLY	N-CA-C	-5.50	102.62	111.59
1	C	351	LEU	N-CA-C	-5.43	105.44	111.36
1	I	144	GLU	N-CA-C	-5.38	106.48	113.16
1	I	140	GLY	N-CA-C	-5.16	103.19	111.59

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	2834	0	2879	47	0
1	B	2840	0	2885	45	4
1	C	2834	0	2879	47	0
1	D	2834	0	2879	45	0
1	E	2842	0	2892	53	0
1	F	2834	0	2879	54	0
1	G	2470	0	2505	44	0
1	H	2834	0	2879	55	0
1	I	2826	0	2867	42	4
1	J	2721	0	2777	53	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	6	0	0	1	0
3	B	6	0	0	0	0
3	C	2	0	0	0	0
3	D	4	0	0	1	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	3	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
All	All	27906	0	28321	457	4

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 8.

All (457) 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:J:51:ALA:HB1	1:J:61:VAL:HG21	1.56	0.88
1:A:196:SER:HA	1:A:284:MET:HE1	1.53	0.88
1:C:139:ALA:H	1:C:182:LYS:HZ3	1.24	0.85
1:J:68:GLN:HB2	1:J:75:GLN:HE21	1.40	0.85
1:A:176:PRO:HG3	1:A:240:GLU:HG3	1.62	0.80
1:G:34:LEU:HD21	1:G:64:PHE:HB2	1.63	0.80
1:H:176:PRO:HG3	1:H:240:GLU:HG2	1.66	0.78
1:F:133:VAL:HG22	1:F:171:VAL:HB	1.65	0.77
1:G:71:PRO:HA	1:G:76:VAL:HG12	1.67	0.76
1:D:32:LYS:HD3	1:D:60:ASP:HB3	1.67	0.76
1:C:133:VAL:HG22	1:C:171:VAL:HB	1.68	0.76
1:D:132:VAL:HG13	1:D:169:PRO:HA	1.70	0.73
1:G:282:VAL:HG21	1:G:342:MET:HE1	1.72	0.72
1:B:133:VAL:HG22	1:B:171:VAL:HB	1.73	0.71
1:J:132:VAL:HG13	1:J:169:PRO:HA	1.73	0.71
1:H:144:GLU:HG2	1:H:145:THR:HG23	1.74	0.70
1:F:35:ILE:HG23	1:F:94:ILE:HD13	1.73	0.70
1:C:32:LYS:HD2	1:C:60:ASP:HB3	1.75	0.69
1:D:176:PRO:HG3	1:D:240:GLU:HG2	1.73	0.69
1:F:54:ILE:HG22	1:F:59:VAL:HB	1.76	0.68
1:A:339:TYR:HA	1:A:342:MET:HE3	1.76	0.67
1:D:115:ARG:HG2	1:D:116:ILE:H	1.58	0.66
1:J:76:VAL:HG21	1:J:151:ILE:HG12	1.77	0.66
1:J:346:GLU:HG3	1:J:349:ILE:HD12	1.77	0.66
1:G:339:TYR:HA	1:G:342:MET:HE3	1.75	0.66
1:J:295:LYS:HE3	1:J:298:ARG:HD3	1.78	0.65
1:F:116:ILE:HD11	1:F:151:ILE:HD13	1.77	0.65
1:E:328:ARG:HA	1:E:331:LYS:HE3	1.79	0.65
1:F:144:GLU:HG2	1:F:145:THR:HG23	1.77	0.65
1:J:80:VAL:HG22	1:J:106:ILE:HA	1.77	0.65
1:J:33:ALA:HB3	1:J:61:VAL:HG12	1.79	0.64
1:C:51:ALA:HB1	1:C:61:VAL:HG21	1.78	0.64
1:B:139:ALA:H	1:B:182:LYS:NZ	1.95	0.64
1:I:133:VAL:HG22	1:I:171:VAL:HB	1.79	0.64
1:C:108:LEU:HD11	1:C:125:VAL:HG21	1.81	0.63
1:A:81:ASP:O	1:A:85:GLN:HG3	1.98	0.63
1:E:133:VAL:HG22	1:E:171:VAL:HB	1.81	0.63
1:H:73:ASP:OD2	1:H:115:ARG:NH2	2.32	0.63
1:G:175:ASP:HB3	1:G:178:LEU:HG	1.81	0.62
1:I:125:VAL:HG12	1:I:166:LYS:HD2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:HIS:NE2	1:A:384:GLU:OE1	2.32	0.62
1:F:127:LYS:HD2	1:F:128:PRO:HD2	1.82	0.62
1:G:213:ALA:HB2	1:F:217:GLN:HG3	1.82	0.62
1:C:139:ALA:H	1:C:182:LYS:NZ	1.96	0.61
1:J:182:LYS:NZ	1:J:190:THR:OG1	2.34	0.61
1:A:283:ASN:HD21	1:A:287:VAL:HG23	1.66	0.61
1:H:120:GLN:HG3	1:H:160:MET:HB3	1.84	0.60
1:B:203:VAL:O	1:B:366:PRO:HG3	2.01	0.60
1:G:144:GLU:HG2	1:G:145:THR:HG23	1.82	0.60
1:A:144:GLU:HG2	1:A:145:THR:HG23	1.84	0.60
1:J:199:ILE:HD12	1:J:284:MET:HE1	1.83	0.60
1:C:50:VAL:O	1:C:54:ILE:HG13	2.02	0.60
1:B:188:ILE:HD13	1:B:333:PHE:HB3	1.84	0.59
1:I:108:LEU:HD11	1:I:125:VAL:HG21	1.83	0.59
1:E:120:GLN:HA	1:E:162:VAL:HG22	1.84	0.59
1:E:14:GLY:HA3	1:I:2:THR:HA	1.85	0.58
1:B:225:TYR:CZ	1:B:241:LYS:HD2	2.37	0.58
1:F:108:LEU:HD11	1:F:125:VAL:HG21	1.84	0.58
1:H:108:LEU:HD11	1:H:125:VAL:HG21	1.85	0.58
1:C:282:VAL:HG21	1:C:342:MET:HE2	1.85	0.58
1:I:42:HIS:CE1	1:I:63:ILE:HG21	2.39	0.58
1:F:15:ARG:HE	1:F:236:ILE:HG12	1.69	0.58
1:I:296:THR:HG22	1:I:315:THR:HG22	1.85	0.58
1:H:138:THR:HB	1:H:190:THR:HG21	1.86	0.57
1:E:140:GLY:N	1:E:246:GLN:HG3	2.19	0.57
1:A:282:VAL:HG21	1:A:342:MET:HE1	1.84	0.57
1:A:261:VAL:HA	1:A:283:ASN:OD1	2.04	0.57
1:J:3:THR:HG21	1:J:208:THR:HG21	1.86	0.57
1:B:261:VAL:HA	1:B:283:ASN:OD1	2.05	0.57
1:G:310:VAL:HA	1:G:313:LEU:HD12	1.86	0.57
1:C:42:HIS:CE1	1:C:63:ILE:HG21	2.39	0.57
1:C:116:ILE:HA	1:C:119:TYR:HD2	1.70	0.57
1:D:346:GLU:CD	1:D:346:GLU:H	2.12	0.57
1:E:142:GLY:HA2	1:E:246:GLN:HE21	1.69	0.56
1:F:47:SER:HB2	1:F:63:ILE:HD13	1.87	0.56
1:E:147:SER:HB3	1:E:168:THR:OG1	2.06	0.56
1:C:144:GLU:HG2	1:C:145:THR:HG23	1.87	0.56
1:F:274:LEU:HD13	1:F:342:MET:HE2	1.87	0.56
1:G:21:VAL:HG13	1:G:22:GLY:H	1.71	0.56
1:G:32:LYS:HE3	1:G:60:ASP:OD2	2.06	0.56
1:G:32:LYS:HG2	1:G:60:ASP:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:SER:HB2	1:B:341:GLU:OE2	2.06	0.56
1:E:199:ILE:HD12	1:E:284:MET:HE1	1.87	0.56
1:E:153:ASP:HB2	1:E:160:MET:HE2	1.88	0.56
1:C:40:PHE:O	1:C:44:THR:HG23	2.06	0.55
1:J:346:GLU:HA	1:J:349:ILE:HG13	1.89	0.55
1:D:136:THR:HG21	1:D:246:GLN:HE22	1.71	0.55
1:E:76:VAL:O	1:E:80:VAL:HG23	2.06	0.55
1:E:208:THR:HG23	1:E:210:VAL:H	1.70	0.55
1:D:112:ASN:HD21	1:D:125:VAL:HG13	1.72	0.55
1:J:54:ILE:HG22	1:J:59:VAL:HB	1.87	0.55
1:C:54:ILE:HG22	1:C:59:VAL:HB	1.87	0.55
1:D:35:ILE:N	1:D:62:ALA:O	2.40	0.55
1:F:73:ASP:CB	1:F:116:ILE:HG21	2.37	0.55
1:B:147:SER:HG	1:B:168:THR:HG1	1.54	0.55
1:F:138:THR:HB	1:F:190:THR:HG21	1.88	0.55
1:H:139:ALA:H	1:H:182:LYS:HZ1	1.55	0.55
1:E:21:VAL:HG13	1:E:22:GLY:H	1.72	0.54
1:B:164:ASP:O	1:B:167:ILE:HG12	2.06	0.54
1:B:274:LEU:HD13	1:B:342:MET:HE2	1.88	0.54
1:H:14:GLY:HA3	1:J:2:THR:HA	1.89	0.54
1:J:345:LYS:NZ	1:J:348:ASP:HB2	2.22	0.54
1:A:298:ARG:NH1	3:A:501:HOH:O	2.41	0.54
1:A:138:THR:HA	1:A:182:LYS:HD2	1.89	0.54
1:E:136:THR:HG22	1:E:138:THR:H	1.72	0.54
1:D:374:ILE:O	1:D:378:ILE:HG13	2.07	0.54
1:J:144:GLU:HG2	1:J:145:THR:HG23	1.90	0.54
1:E:24:ARG:NH1	1:I:165:GLU:OE2	2.38	0.54
1:J:64:PHE:CZ	1:J:79:GLY:HA2	2.42	0.54
1:E:274:LEU:HD13	1:E:342:MET:HE2	1.90	0.54
1:F:104:LYS:HD3	1:F:167:ILE:HD12	1.90	0.54
1:E:120:GLN:NE2	1:E:160:MET:HB2	2.24	0.53
1:A:133:VAL:HG22	1:A:171:VAL:HB	1.90	0.53
1:H:346:GLU:H	1:H:346:GLU:CD	2.15	0.53
1:D:40:PHE:O	1:D:44:THR:HG23	2.09	0.53
1:B:138:THR:HB	1:B:190:THR:HG21	1.91	0.53
1:E:115:ARG:HG2	1:E:117:ASN:H	1.74	0.53
1:B:115:ARG:CZ	1:B:117:ASN:HB2	2.38	0.53
1:D:217:GLN:HG2	3:D:502:HOH:O	2.09	0.53
1:H:274:LEU:HD13	1:H:342:MET:HE2	1.91	0.53
1:J:297:GLU:CD	1:J:297:GLU:H	2.16	0.53
1:C:339:TYR:HD1	1:C:342:MET:HE3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:HB	1:A:190:THR:HG21	1.91	0.53
1:H:76:VAL:O	1:H:80:VAL:HG23	2.09	0.52
1:H:199:ILE:HG23	1:H:302:ILE:HD13	1.90	0.52
1:J:7:ILE:HD12	1:J:251:VAL:HG11	1.91	0.52
1:A:125:VAL:HG12	1:A:166:LYS:HD2	1.89	0.52
1:C:339:TYR:CD1	1:C:342:MET:HE3	2.45	0.52
1:E:182:LYS:HE3	1:E:186:LEU:HG	1.91	0.52
1:E:199:ILE:HD11	1:E:306:LEU:HD11	1.91	0.52
1:D:21:VAL:HG11	1:D:50:VAL:HG13	1.92	0.52
1:E:55:ARG:HA	1:E:59:VAL:O	2.10	0.52
1:H:210:VAL:HG23	1:J:244:TYR:HD1	1.75	0.52
1:C:120:GLN:HB2	1:C:160:MET:HE2	1.91	0.52
1:I:297:GLU:H	1:I:297:GLU:CD	2.18	0.52
1:H:200:GLU:CD	1:H:261:VAL:HB	2.35	0.52
1:G:250:GLY:HA2	1:G:253:PHE:CD2	2.45	0.51
1:H:30:ALA:HB1	1:H:90:SER:HB3	1.92	0.51
1:I:92:VAL:HG22	1:I:133:VAL:HB	1.91	0.51
1:J:351:LEU:H	1:J:351:LEU:HD12	1.76	0.51
1:G:54:ILE:HG22	1:G:59:VAL:HB	1.93	0.51
1:C:5:PHE:HB3	1:A:11:SER:HB2	1.93	0.51
1:J:35:ILE:HG23	1:J:94:ILE:HD13	1.92	0.51
1:G:261:VAL:HG21	1:G:284:MET:HG3	1.91	0.51
1:I:51:ALA:HB1	1:I:61:VAL:HG21	1.91	0.51
1:H:13:ILE:HG23	1:H:174:VAL:HB	1.92	0.51
1:B:71:PRO:O	1:B:152:THR:HG22	2.10	0.51
1:E:298:ARG:O	1:E:302:ILE:HG13	2.11	0.51
1:I:77:HIS:CE1	1:I:115:ARG:HA	2.46	0.51
1:H:308:GLU:OE1	1:H:321:ARG:NH2	2.43	0.51
1:J:7:ILE:HG13	1:J:8:PRO:HD2	1.92	0.51
1:F:50:VAL:O	1:F:54:ILE:HG13	2.10	0.51
1:J:133:VAL:HG22	1:J:171:VAL:HB	1.94	0.50
1:B:139:ALA:H	1:B:182:LYS:HZ2	1.59	0.50
1:F:140:GLY:O	1:F:142:GLY:N	2.39	0.50
1:H:153:ASP:HB2	1:H:160:MET:SD	2.51	0.50
1:B:212:ASP:CG	1:B:298:ARG:HH22	2.19	0.50
1:C:116:ILE:HD11	1:C:162:VAL:HG11	1.94	0.50
1:C:138:THR:HB	1:C:190:THR:HG21	1.93	0.50
1:A:108:LEU:HD11	1:A:125:VAL:HG21	1.94	0.50
1:A:174:VAL:CG1	1:A:243:ALA:HB1	2.42	0.50
1:H:139:ALA:H	1:H:182:LYS:NZ	2.09	0.50
1:E:260:LEU:HA	1:E:263:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:VAL:CG2	1:G:78:GLU:HG3	2.42	0.50
1:I:73:ASP:OD1	1:I:73:ASP:N	2.41	0.50
1:B:138:THR:HA	1:B:182:LYS:HD2	1.93	0.50
1:B:250:GLY:HA2	1:B:253:PHE:CE2	2.47	0.50
1:F:100:HIS:O	1:F:104:LYS:HG2	2.12	0.50
1:C:15:ARG:HD3	1:A:1:MET:HG3	1.94	0.49
1:H:34:LEU:HB2	1:H:88:CYS:SG	2.52	0.49
1:J:313:LEU:HB3	1:J:317:ALA:HB3	1.93	0.49
1:G:83:PHE:HZ	1:G:91:LEU:HD11	1.76	0.49
1:G:350:GLU:O	1:G:354:LYS:HG2	2.12	0.49
1:H:64:PHE:CZ	1:H:66:LYS:HD3	2.47	0.49
1:I:54:ILE:HG22	1:I:59:VAL:HB	1.95	0.49
1:D:139:ALA:H	1:D:182:LYS:NZ	2.11	0.49
1:A:78:GLU:O	1:A:82:VAL:HG23	2.12	0.49
1:E:272:TYR:CE2	1:E:344:VAL:HA	2.47	0.49
1:F:3:THR:HG21	1:F:208:THR:HG21	1.93	0.49
1:I:348:ASP:HA	1:I:351:LEU:HD13	1.94	0.49
1:J:373:ASP:O	1:J:377:ILE:HG13	2.12	0.49
1:E:33:ALA:O	1:E:61:VAL:HA	2.12	0.49
1:H:42:HIS:HD2	1:H:65:PRO:HG3	1.78	0.49
1:E:7:ILE:HD13	1:I:7:ILE:HG21	1.95	0.48
1:E:140:GLY:O	1:E:142:GLY:N	2.39	0.48
1:F:40:PHE:O	1:F:44:THR:HG23	2.12	0.48
1:J:280:ASN:O	1:J:284:MET:HG3	2.14	0.48
1:F:72:ALA:HA	1:F:152:THR:HG22	1.95	0.48
1:D:278:ILE:O	1:D:282:VAL:HG23	2.12	0.48
1:F:81:ASP:O	1:F:85:GLN:HG2	2.13	0.48
1:I:76:VAL:O	1:I:80:VAL:HG23	2.14	0.48
1:J:12:VAL:HB	1:J:173:ILE:HD13	1.94	0.48
1:E:129:VAL:HG22	1:E:166:LYS:HB3	1.96	0.48
1:D:140:GLY:O	1:D:142:GLY:N	2.43	0.48
1:D:261:VAL:HG21	1:D:284:MET:HG2	1.96	0.48
1:H:148:LEU:HB2	1:H:163:ILE:HG12	1.96	0.48
1:G:100:HIS:O	1:G:104:LYS:HG2	2.13	0.48
1:H:80:VAL:HG22	1:H:106:ILE:HA	1.96	0.48
1:J:21:VAL:HG21	1:J:50:VAL:HG13	1.96	0.48
1:J:278:ILE:O	1:J:282:VAL:HG23	2.14	0.48
1:F:374:ILE:O	1:F:378:ILE:HG13	2.14	0.48
1:C:236:ILE:O	1:C:240:GLU:HG3	2.13	0.48
1:A:250:GLY:HA2	1:A:253:PHE:CE2	2.48	0.48
1:A:21:VAL:HG13	1:A:22:GLY:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:40:PHE:O	1:J:44:THR:HG23	2.13	0.47
1:E:297:GLU:CD	1:E:297:GLU:H	2.22	0.47
1:C:7:ILE:HG13	1:C:8:PRO:HD2	1.95	0.47
1:I:138:THR:HG22	1:I:182:LYS:HD3	1.96	0.47
1:E:78:GLU:O	1:E:82:VAL:HG23	2.14	0.47
1:G:136:THR:HG22	1:G:138:THR:H	1.79	0.47
1:F:93:SER:OG	1:F:100:HIS:HA	2.13	0.47
1:D:184:ALA:O	1:D:188:ILE:HG13	2.15	0.47
1:J:76:VAL:O	1:J:80:VAL:HG23	2.14	0.47
1:E:200:GLU:CD	1:E:261:VAL:HB	2.39	0.47
1:G:64:PHE:CZ	1:G:66:LYS:HB3	2.49	0.47
1:H:73:ASP:HB3	1:H:116:ILE:HG21	1.96	0.47
1:J:345:LYS:HZ2	1:J:348:ASP:HB2	1.79	0.47
1:G:21:VAL:HG13	1:G:22:GLY:N	2.30	0.47
1:G:250:GLY:HA2	1:G:253:PHE:CE2	2.49	0.47
1:I:77:HIS:HE1	1:I:115:ARG:HA	1.79	0.47
1:B:76:VAL:O	1:B:80:VAL:HG23	2.15	0.47
1:E:40:PHE:O	1:E:44:THR:HG23	2.14	0.47
1:G:139:ALA:H	1:G:182:LYS:NZ	2.13	0.47
1:F:80:VAL:HG22	1:F:106:ILE:HA	1.97	0.47
1:D:12:VAL:HB	1:D:173:ILE:HD13	1.97	0.47
1:D:24:ARG:O	1:D:28:ILE:HG13	2.14	0.47
1:H:15:ARG:O	1:J:2:THR:OG1	2.32	0.47
1:E:139:ALA:H	1:E:182:LYS:NZ	2.13	0.47
1:F:351:LEU:HD12	1:F:351:LEU:H	1.79	0.47
1:B:85:GLN:HG3	1:B:86:GLU:HG2	1.97	0.47
1:H:310:VAL:HA	1:H:313:LEU:HD12	1.97	0.47
1:A:20:GLU:O	1:A:24:ARG:HG3	2.15	0.47
1:D:112:ASN:HB3	1:D:119:TYR:OH	2.14	0.46
1:G:76:VAL:HG23	1:G:78:GLU:HG3	1.97	0.46
1:H:64:PHE:CZ	1:H:79:GLY:HA2	2.50	0.46
1:C:77:HIS:NE2	1:C:115:ARG:HA	2.31	0.46
1:F:64:PHE:HZ	1:F:78:GLU:HG2	1.80	0.46
1:I:50:VAL:O	1:I:54:ILE:HG13	2.15	0.46
1:I:250:GLY:HA2	1:I:253:PHE:CE2	2.51	0.46
1:J:350:GLU:O	1:J:354:LYS:HG3	2.15	0.46
1:I:26:LYS:HA	1:I:26:LYS:HD2	1.42	0.46
1:B:297:GLU:H	1:B:297:GLU:CD	2.22	0.46
1:D:375:ALA:O	1:D:379:LYS:HG3	2.16	0.46
1:J:296:THR:HG22	1:J:315:THR:HG22	1.97	0.46
1:E:148:LEU:HD13	1:E:163:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:VAL:HG23	1:G:287:VAL:HG11	1.98	0.46
1:F:76:VAL:HG21	1:F:151:ILE:HG12	1.98	0.46
1:B:42:HIS:CE1	1:B:63:ILE:HG21	2.51	0.46
1:E:276:HIS:CE1	1:E:280:ASN:HD21	2.33	0.46
1:G:34:LEU:HD22	1:G:83:PHE:CD1	2.50	0.46
1:I:28:ILE:HD11	1:I:171:VAL:HG23	1.98	0.46
1:H:40:PHE:O	1:H:44:THR:HG23	2.16	0.46
1:C:217:GLN:HG3	1:A:213:ALA:HB2	1.98	0.46
1:H:148:LEU:HD21	1:H:150:VAL:HG23	1.97	0.46
1:I:100:HIS:O	1:I:104:LYS:HG3	2.16	0.46
1:H:23:THR:OG1	1:H:24:ARG:N	2.49	0.45
1:C:138:THR:HA	1:C:182:LYS:HD2	1.97	0.45
1:C:176:PRO:HG3	1:C:240:GLU:HG2	1.99	0.45
1:I:351:LEU:HD12	1:I:351:LEU:H	1.80	0.45
1:E:15[A]:ARG:HE	1:E:15[A]:ARG:HB3	1.54	0.45
1:C:208:THR:HG23	1:C:211:THR:H	1.81	0.45
1:A:351:LEU:HD12	1:A:351:LEU:H	1.81	0.45
1:E:272:TYR:CZ	1:E:344:VAL:HA	2.52	0.45
1:F:74:THR:HA	1:F:77:HIS:CE1	2.52	0.45
1:F:116:ILE:HG12	1:F:151:ILE:HG21	1.98	0.45
1:A:346:GLU:H	1:A:346:GLU:CD	2.24	0.45
1:B:54:ILE:HG23	1:B:59:VAL:HB	1.99	0.45
1:H:213:ALA:HA	1:J:217:GLN:HG3	1.97	0.45
1:I:18:VAL:O	1:I:21:VAL:HG22	2.17	0.45
1:I:147:SER:HB3	1:I:164:ASP:O	2.17	0.45
1:H:174:VAL:HG12	1:H:243:ALA:HB1	1.99	0.45
1:E:21:VAL:HG11	1:E:50:VAL:HG13	1.99	0.45
1:C:375:ALA:HA	1:C:378:ILE:HD12	1.99	0.45
1:A:64:PHE:CZ	1:A:66:LYS:HB2	2.52	0.45
1:D:112:ASN:ND2	1:D:127:LYS:HB2	2.32	0.45
1:D:226:LEU:N	1:D:227:PRO:HD2	2.32	0.45
1:H:7:ILE:HG13	1:H:8:PRO:HD2	1.98	0.45
1:D:140:GLY:N	1:D:246:GLN:HG3	2.32	0.45
1:E:261:VAL:HG21	1:E:284:MET:HG2	1.99	0.45
1:C:82:VAL:O	1:C:86:GLU:HG2	2.17	0.45
1:J:246:GLN:HG3	1:J:247:TYR:N	2.32	0.45
1:E:317:ALA:O	1:E:321:ARG:HG2	2.16	0.45
1:G:36:VAL:HA	1:G:64:PHE:HB3	1.99	0.45
1:F:73:ASP:HB3	1:F:116:ILE:HG21	1.99	0.45
1:H:64:PHE:CE2	1:H:66:LYS:HB2	2.52	0.44
1:E:217:GLN:HG3	1:I:213:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ALA:H	1:A:182:LYS:NZ	2.15	0.44
1:H:78:GLU:O	1:H:82:VAL:HG23	2.17	0.44
1:J:64:PHE:CZ	1:J:66:LYS:HB2	2.53	0.44
1:G:7:ILE:HG13	1:G:8:PRO:HD2	1.99	0.44
1:G:336:PRO:HB2	1:G:342:MET:HE2	1.98	0.44
1:F:76:VAL:HG11	1:F:116:ILE:HD13	1.99	0.44
1:D:373:ASP:O	1:D:377:ILE:HG13	2.17	0.44
1:G:374:ILE:O	1:G:378:ILE:HG13	2.17	0.44
1:I:83:PHE:CZ	1:I:130:VAL:HG11	2.52	0.44
1:H:100:HIS:HE2	1:H:136:THR:HA	1.81	0.44
1:E:289:ALA:HA	1:E:292:LEU:HD13	1.98	0.44
1:E:342:MET:HE2	1:E:342:MET:HB3	1.89	0.44
1:C:142:GLY:O	1:C:146:THR:HG23	2.17	0.44
1:A:282:VAL:HG21	1:A:342:MET:CE	2.48	0.44
1:J:42:HIS:CD2	1:J:63:ILE:HG21	2.53	0.44
1:B:139:ALA:H	1:B:182:LYS:HZ3	1.65	0.44
1:A:221:LEU:HD22	1:A:241:LYS:HB3	1.99	0.44
1:H:317:ALA:O	1:H:321:ARG:HG2	2.18	0.44
1:H:203:VAL:HG11	1:H:299:PHE:CZ	2.53	0.44
1:H:210:VAL:HG23	1:J:244:TYR:CD1	2.53	0.44
1:J:26:LYS:HA	1:J:26:LYS:HD2	1.89	0.44
1:C:217:GLN:HG3	1:A:213:ALA:CB	2.48	0.44
1:C:263:SER:OG	1:C:361:CYS:HB2	2.17	0.44
1:A:25:LEU:HD11	1:A:92:VAL:HG21	2.00	0.44
1:I:13:ILE:HG23	1:I:174:VAL:HB	1.98	0.44
1:I:41:LEU:HD13	1:I:46:LEU:HD23	2.00	0.44
1:I:383:LEU:HD23	1:I:383:LEU:HA	1.91	0.44
1:B:370:THR:O	1:B:374:ILE:HG13	2.18	0.43
1:C:247:TYR:O	1:C:251:VAL:HG23	2.16	0.43
1:A:268:VAL:HG12	1:A:274:LEU:HD12	2.00	0.43
1:B:2:THR:HA	1:D:14:GLY:HA3	1.99	0.43
1:B:80:VAL:O	1:B:84:LYS:HG2	2.18	0.43
1:H:82:VAL:O	1:H:86:GLU:HG2	2.18	0.43
1:G:50:VAL:O	1:G:54:ILE:HG13	2.18	0.43
1:F:363:GLN:N	1:F:363:GLN:OE1	2.51	0.43
1:C:298:ARG:O	1:C:302:ILE:HG13	2.18	0.43
1:B:292:LEU:HD12	1:B:299:PHE:CD2	2.53	0.43
1:F:152:THR:HA	1:F:159:LYS:HA	1.99	0.43
1:F:195:LEU:O	1:F:199:ILE:HG13	2.18	0.43
1:A:339:TYR:HB2	1:A:382:MET:HA	2.01	0.43
1:B:209:PRO:HB3	1:D:221:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:MET:HG2	1:A:326:LEU:HD13	2.00	0.43
1:I:250:GLY:HA2	1:I:253:PHE:CD2	2.54	0.43
1:J:166:LYS:HD2	1:J:166:LYS:HA	1.87	0.43
1:I:295:LYS:HE3	1:I:298:ARG:HD2	1.99	0.43
1:D:51:ALA:HB1	1:D:61:VAL:HG21	2.00	0.43
1:D:73:ASP:O	1:D:76:VAL:HG22	2.17	0.43
1:E:4:ASN:OD1	1:I:12:VAL:HG22	2.19	0.43
1:E:195:LEU:HD13	1:E:222:ILE:HG21	2.01	0.43
1:F:112:ASN:OD1	1:F:125:VAL:HG13	2.18	0.43
1:C:2:THR:HA	1:A:14:GLY:HA3	1.99	0.43
1:D:25:LEU:HD12	1:D:25:LEU:HA	1.85	0.43
1:H:76:VAL:HG11	1:H:116:ILE:HD13	2.00	0.43
1:G:15:ARG:O	1:F:2:THR:OG1	2.34	0.43
1:B:5:PHE:HB3	1:D:11:SER:HB2	2.00	0.43
1:E:12:VAL:HG11	1:E:20:GLU:HG3	1.99	0.43
1:C:63:ILE:HG22	1:C:65:PRO:HD3	2.01	0.43
1:A:261:VAL:HG23	1:A:287:VAL:HG11	2.01	0.43
1:A:345:LYS:HB3	1:A:347:GLU:HG2	2.01	0.43
1:J:142:GLY:O	1:J:146:THR:HG23	2.19	0.43
1:F:297:GLU:CD	1:F:297:GLU:H	2.27	0.43
1:B:195:LEU:HD13	1:B:222:ILE:HG21	2.01	0.42
1:C:221:LEU:HD22	1:C:241:LYS:HB3	2.00	0.42
1:A:71:PRO:O	1:A:152:THR:HG22	2.18	0.42
1:J:64:PHE:CE1	1:J:66:LYS:HD2	2.53	0.42
1:G:213:ALA:CB	1:F:217:GLN:HG3	2.47	0.42
1:I:292:LEU:HA	1:I:292:LEU:HD23	1.81	0.42
1:D:337:SER:HB2	1:D:341:GLU:OE2	2.19	0.42
1:B:25:LEU:HD12	1:B:25:LEU:HA	1.78	0.42
1:A:164:ASP:O	1:A:167:ILE:HG12	2.19	0.42
1:B:71:PRO:HG2	1:B:150:VAL:O	2.19	0.42
1:D:112:ASN:HD22	1:D:127:LYS:HB2	1.84	0.42
1:B:263:SER:OG	1:B:361:CYS:HB2	2.19	0.42
1:H:133:VAL:HG22	1:H:171:VAL:HB	2.01	0.42
1:J:317:ALA:O	1:J:321:ARG:HG2	2.19	0.42
1:G:182:LYS:HD2	1:G:186:LEU:HG	2.02	0.42
1:F:32:LYS:HB2	1:F:89:ASP:H	1.84	0.42
1:F:26:LYS:HD2	1:F:26:LYS:HA	1.69	0.42
1:I:41:LEU:HD23	1:I:41:LEU:HA	1.84	0.42
1:J:143:SER:C	1:J:145:THR:H	2.26	0.42
1:F:260:LEU:HD21	1:F:374:ILE:HG12	2.02	0.42
1:C:83:PHE:CE1	1:C:91:LEU:HG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:373:ASP:O	1:G:377:ILE:HG13	2.20	0.41
1:A:35:ILE:HA	1:A:92:VAL:O	2.20	0.41
1:B:341:GLU:H	1:B:341:GLU:HG3	1.69	0.41
1:E:80:VAL:HG22	1:E:106:ILE:HA	2.01	0.41
1:F:50:VAL:HG12	1:F:54:ILE:HD11	2.02	0.41
1:C:117:ASN:HA	1:C:160:MET:HE1	2.01	0.41
1:B:21:VAL:HG13	1:B:22:GLY:H	1.85	0.41
1:B:225:TYR:CE1	1:B:241:LYS:HD2	2.55	0.41
1:B:340:ALA:HB2	1:B:382:MET:HE3	2.02	0.41
1:D:156:ARG:O	1:D:158:VAL:HG23	2.19	0.41
1:H:33:ALA:O	1:H:61:VAL:HA	2.20	0.41
1:G:228:LYS:NZ	1:I:294:ALA:O	2.53	0.41
1:C:78:GLU:O	1:C:82:VAL:HG23	2.20	0.41
1:D:64:PHE:CD1	1:D:82:VAL:HG21	2.55	0.41
1:D:139:ALA:H	1:D:182:LYS:HZ2	1.68	0.41
1:J:199:ILE:HD12	1:J:284:MET:CE	2.50	0.41
1:E:208:THR:HG22	1:E:211:THR:H	1.85	0.41
1:I:382:MET:HE3	1:I:382:MET:HB3	1.90	0.41
1:H:73:ASP:HA	1:H:76:VAL:HB	2.01	0.41
1:F:41:LEU:HD23	1:F:41:LEU:HA	1.90	0.41
1:I:83:PHE:HZ	1:I:130:VAL:HG11	1.85	0.41
1:H:45:GLY:O	1:H:49:GLU:HG3	2.21	0.41
1:J:34:LEU:HD12	1:J:62:ALA:HB3	2.02	0.41
1:G:217:GLN:HG3	1:F:213:ALA:HA	2.03	0.41
1:B:40:PHE:O	1:B:44:THR:HG23	2.21	0.41
1:D:144:GLU:HG2	1:D:145:THR:HG23	2.02	0.41
1:H:258:LEU:HB3	1:H:259:GLY:H	1.62	0.41
1:G:130:VAL:HA	1:G:131:PRO:HD3	1.90	0.41
1:G:181:LYS:HA	1:G:181:LYS:HD3	1.87	0.41
1:A:122:VAL:HA	1:A:163:ILE:HB	2.01	0.41
1:A:373:ASP:O	1:A:377:ILE:HG13	2.21	0.41
1:D:111:ALA:HB1	1:D:127:LYS:HB3	2.03	0.41
1:H:32:LYS:HE2	1:H:88:CYS:SG	2.61	0.41
1:H:64:PHE:CE1	1:H:66:LYS:HD3	2.55	0.41
1:E:21:VAL:HG13	1:E:22:GLY:N	2.36	0.41
1:F:23:THR:O	1:F:27:GLN:HG3	2.20	0.41
1:B:152:THR:HA	1:B:159:LYS:HA	2.03	0.41
1:B:236:ILE:HD12	1:B:236:ILE:HA	1.94	0.41
1:B:310:VAL:HA	1:B:313:LEU:HD12	2.02	0.41
1:H:214:PHE:CZ	1:J:210:VAL:HG13	2.56	0.41
1:H:236:ILE:HD12	1:H:236:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:PHE:CZ	1:E:66:LYS:HB2	2.56	0.41
1:E:213:ALA:HA	1:I:217:GLN:HG3	2.02	0.41
1:E:337:SER:HB2	1:E:341:GLU:OE2	2.21	0.41
1:G:297:GLU:H	1:G:297:GLU:CD	2.29	0.41
1:G:349:ILE:HD13	1:G:379:LYS:HG2	2.03	0.41
1:F:34:LEU:HB3	1:F:91:LEU:HD23	2.02	0.41
1:F:66:LYS:NZ	1:F:78:GLU:OE2	2.54	0.41
1:F:197:HIS:HB2	1:F:249:ALA:HB1	2.03	0.41
1:F:383:LEU:O	1:F:384:GLU:HB2	2.20	0.41
1:C:6:PHE:CE2	1:C:165:GLU:HB2	2.56	0.41
1:B:253:PHE:CD1	1:B:253:PHE:C	2.98	0.41
1:H:94:ILE:HG12	1:H:135:ILE:HD12	2.02	0.41
1:H:197:HIS:CD2	1:H:262:HIS:CE1	3.09	0.41
1:J:182:LYS:HE2	1:J:182:LYS:HB3	1.81	0.41
1:G:136:THR:HG21	1:G:246:GLN:HE22	1.85	0.41
1:G:296:THR:HG22	1:G:315:THR:HG22	2.02	0.41
1:F:313:LEU:HD23	1:F:313:LEU:HA	1.95	0.41
1:C:382:MET:HE3	1:C:382:MET:HB3	1.99	0.41
1:A:250:GLY:HA2	1:A:253:PHE:CD2	2.55	0.41
1:A:375:ALA:O	1:A:379:LYS:HG3	2.21	0.41
1:E:261:VAL:HG23	1:E:287:VAL:HG11	2.04	0.40
1:F:260:LEU:HA	1:F:263:SER:HB2	2.03	0.40
1:C:153:ASP:O	1:C:157:LYS:N	2.54	0.40
1:I:157:LYS:HA	1:I:157:LYS:HD3	1.66	0.40
1:B:213:ALA:HB2	1:D:217:GLN:HG3	2.03	0.40
1:B:226:LEU:N	1:B:227:PRO:HD2	2.37	0.40
1:H:374:ILE:O	1:H:378:ILE:HG13	2.20	0.40
1:C:226:LEU:O	1:C:230:VAL:HG23	2.22	0.40
1:A:205:LYS:HG2	1:A:366:PRO:HA	2.04	0.40
1:A:260:LEU:HD23	1:A:362:THR:HG22	2.03	0.40
1:B:14:GLY:HA3	1:D:2:THR:HA	2.03	0.40
1:D:142:GLY:O	1:D:146:THR:HG23	2.21	0.40
1:D:151:ILE:O	1:D:160:MET:HG3	2.21	0.40
1:D:378:ILE:O	1:D:382:MET:HG2	2.22	0.40
1:H:383:LEU:HD23	1:H:383:LEU:HA	1.83	0.40
1:E:138:THR:HB	1:E:190:THR:HG21	2.03	0.40
1:F:139:ALA:H	1:F:182:LYS:NZ	2.20	0.40
1:C:217:GLN:HG3	1:A:213:ALA:HA	2.03	0.40
1:I:260:LEU:HA	1:I:263:SER:HB2	2.04	0.40
1:J:83:PHE:CZ	1:J:88:CYS:HB2	2.56	0.40
1:F:73:ASP:OD1	1:F:73:ASP:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:LEU:HA	1:C:41:LEU:HD23	1.86	0.40
1:C:72:ALA:HA	1:C:152:THR:HG22	2.04	0.40
1:D:73:ASP:HA	1:D:76:VAL:HG22	2.03	0.40
1:D:157:LYS:HE3	1:D:157:LYS:HB2	1.94	0.40
1:J:33:ALA:HA	1:J:90:SER:O	2.21	0.40
1:G:129:VAL:HG22	1:G:166:LYS:HE3	2.03	0.40
1:F:373:ASP:O	1:F:377:ILE:HG13	2.21	0.40

All (4) 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:115:ARG:CZ	1:I:26:LYS:NZ[3_554]	1.33	0.87
1:B:115:ARG:NH1	1:I:26:LYS:NZ[3_554]	1.48	0.72
1:B:115:ARG:NE	1:I:26:LYS:NZ[3_554]	1.93	0.27
1:B:115:ARG:NH2	1:I:26:LYS:NZ[3_554]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/390 (98%)	365 (96%)	17 (4%)	0	100	100
1	B	383/390 (98%)	370 (97%)	13 (3%)	0	100	100
1	C	382/390 (98%)	371 (97%)	11 (3%)	0	100	100
1	D	382/390 (98%)	364 (95%)	18 (5%)	0	100	100
1	E	383/390 (98%)	366 (96%)	15 (4%)	2 (0%)	24	60
1	F	382/390 (98%)	362 (95%)	20 (5%)	0	100	100
1	G	325/390 (83%)	313 (96%)	12 (4%)	0	100	100
1	H	382/390 (98%)	366 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	381/390 (98%)	366 (96%)	14 (4%)	1 (0%)	36	70
1	J	363/390 (93%)	343 (94%)	18 (5%)	2 (1%)	21	56
All	All	3745/3900 (96%)	3586 (96%)	154 (4%)	5 (0%)	48	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	141	THR
1	I	141	THR
1	J	70	ASP
1	J	256	GLY
1	E	65	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/306 (98%)	294 (98%)	6 (2%)	48	76
1	B	301/306 (98%)	296 (98%)	5 (2%)	53	78
1	C	300/306 (98%)	287 (96%)	13 (4%)	26	60
1	D	300/306 (98%)	291 (97%)	9 (3%)	36	69
1	E	301/306 (98%)	292 (97%)	9 (3%)	36	69
1	F	300/306 (98%)	288 (96%)	12 (4%)	28	62
1	G	260/306 (85%)	256 (98%)	4 (2%)	57	80
1	H	300/306 (98%)	294 (98%)	6 (2%)	48	76
1	I	299/306 (98%)	287 (96%)	12 (4%)	28	62
1	J	289/306 (94%)	274 (95%)	15 (5%)	21	55
All	All	2950/3060 (96%)	2859 (97%)	91 (3%)	35	68

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	LEU
1	B	127	LYS
1	B	129	VAL
1	B	236	ILE
1	B	246	GLN
1	D	19	LYS
1	D	23	THR
1	D	112	ASN
1	D	123	ASN
1	D	129	VAL
1	D	136	THR
1	D	292	LEU
1	D	320	GLU
1	D	349	ILE
1	H	63	ILE
1	H	129	VAL
1	H	143	SER
1	H	148	LEU
1	H	160	MET
1	H	253	PHE
1	J	23	THR
1	J	25	LEU
1	J	32	LYS
1	J	47	SER
1	J	68	GLN
1	J	70	ASP
1	J	73	ASP
1	J	102	THR
1	J	109	VAL
1	J	132	VAL
1	J	147	SER
1	J	148	LEU
1	J	174	VAL
1	J	246	GLN
1	J	292	LEU
1	E	15[A]	ARG
1	E	15[B]	ARG
1	E	31	LYS
1	E	118	ASP
1	E	125	VAL
1	E	147	SER
1	E	208	THR
1	E	292	LEU

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Mol	Chain	Res	Type
1	E	341	GLU
1	G	3	THR
1	G	99	SER
1	G	292	LEU
1	G	345	LYS
1	F	21	VAL
1	F	23	THR
1	F	24	ARG
1	F	26	LYS
1	F	35	ILE
1	F	122	VAL
1	F	125	VAL
1	F	129	VAL
1	F	154	SER
1	F	246	GLN
1	F	281	SER
1	F	292	LEU
1	C	21	VAL
1	C	118	ASP
1	C	122	VAL
1	C	125	VAL
1	C	150	VAL
1	C	152	THR
1	C	156	ARG
1	C	342	MET
1	C	346	GLU
1	C	349	ILE
1	C	350	GLU
1	C	351	LEU
1	C	383	LEU
1	A	125	VAL
1	A	129	VAL
1	A	147	SER
1	A	173	ILE
1	A	246	GLN
1	A	292	LEU
1	I	2	THR
1	I	21	VAL
1	I	24	ARG
1	I	26	LYS
1	I	125	VAL
1	I	136	THR

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Mol	Chain	Res	Type
1	I	138	THR
1	I	141	THR
1	I	143	SER
1	I	145	THR
1	I	350	GLU
1	I	370	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	ASN
1	B	283	ASN
1	B	363	GLN
1	D	112	ASN
1	D	123	ASN
1	H	123	ASN
1	H	232	ASN
1	H	286	HIS
1	H	330	ASN
1	J	75	GLN
1	J	85	GLN
1	J	123	ASN
1	J	223	ASN
1	J	266	HIS
1	J	275	GLN
1	J	283	ASN
1	E	120	GLN
1	E	223	ASN
1	E	246	GLN
1	G	85	GLN
1	G	223	ASN
1	G	232	ASN
1	G	280	ASN
1	G	330	ASN
1	F	68	GLN
1	F	123	ASN
1	C	123	ASN
1	C	223	ASN
1	C	283	ASN
1	A	87	ASN
1	I	68	GLN
1	I	117	ASN

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Mol	Chain	Res	Type
1	I	232	ASN
1	I	267	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	384/390 (98%)	-0.46	1 (0%) 90 79	31, 51, 69, 93	0
1	B	384/390 (98%)	-0.46	2 (0%) 87 72	31, 48, 71, 96	1 (0%)
1	C	384/390 (98%)	-0.36	0 100 100	33, 55, 80, 106	0
1	D	384/390 (98%)	-0.17	3 (0%) 82 64	34, 54, 103, 115	0
1	E	384/390 (98%)	-0.24	4 (1%) 79 59	32, 54, 96, 131	1 (0%)
1	F	384/390 (98%)	-0.04	11 (2%) 53 31	34, 57, 115, 129	0
1	G	335/390 (85%)	-0.25	4 (1%) 76 55	31, 52, 112, 146	0
1	H	384/390 (98%)	-0.11	9 (2%) 61 38	36, 60, 119, 138	0
1	I	383/390 (98%)	-0.40	0 100 100	31, 47, 80, 110	0
1	J	369/390 (94%)	0.08	19 (5%) 33 17	40, 64, 137, 158	0
All	All	3775/3900 (96%)	-0.24	53 (1%) 73 51	31, 53, 110, 158	2 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	83	PHE	5.5
1	F	108	LEU	4.7
1	G	105	ALA	3.9
1	J	160	MET	3.9
1	J	161	PRO	3.9
1	J	34	LEU	3.8
1	E	116	ILE	3.8
1	J	162	VAL	3.7
1	F	34	LEU	3.5
1	J	150	VAL	3.4
1	D	116	ILE	3.3
1	B	1	MET	3.2
1	F	88	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	90	SER	3.1
1	F	70	ASP	3.1
1	F	2	THR	2.8
1	J	111	ALA	2.8
1	J	110	ALA	2.8
1	J	151	ILE	2.7
1	H	108	LEU	2.7
1	H	122	VAL	2.6
1	E	153	ASP	2.6
1	F	162	VAL	2.6
1	H	116	ILE	2.5
1	A	1	MET	2.5
1	J	67	ALA	2.5
1	H	152	THR	2.5
1	J	38	ASP	2.5
1	J	91	LEU	2.5
1	G	70	ASP	2.4
1	F	107	GLY	2.4
1	J	105	ALA	2.4
1	J	163	ILE	2.4
1	J	70	ASP	2.4
1	E	158	VAL	2.4
1	J	106	ILE	2.4
1	B	49	GLU	2.4
1	F	105	ALA	2.3
1	H	128	PRO	2.3
1	J	88	CYS	2.3
1	J	109	VAL	2.3
1	F	91	LEU	2.3
1	D	109	VAL	2.2
1	H	158	VAL	2.2
1	F	158	VAL	2.1
1	E	161	PRO	2.1
1	H	63	ILE	2.1
1	J	149	ALA	2.1
1	F	109	VAL	2.1
1	H	161	PRO	2.1
1	G	45	GLY	2.0
1	H	151	ILE	2.0
1	D	161	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	E	401	1/1	0.96	0.05	38,38,38,38	0
2	MN	H	401	1/1	0.97	0.05	43,43,43,43	0
2	MN	J	401	1/1	0.98	0.05	52,52,52,52	0
2	MN	B	401	1/1	0.98	0.04	40,40,40,40	0
2	MN	F	401	1/1	0.98	0.05	48,48,48,48	0
2	MN	I	401	1/1	0.98	0.05	43,43,43,43	0
2	MN	D	401	1/1	0.99	0.03	46,46,46,46	0
2	MN	C	401	1/1	0.99	0.03	46,46,46,46	0
2	MN	A	401	1/1	0.99	0.03	47,47,47,47	0
2	MN	G	401	1/1	0.99	0.04	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.