



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2025 – 02:23 PM JST

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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

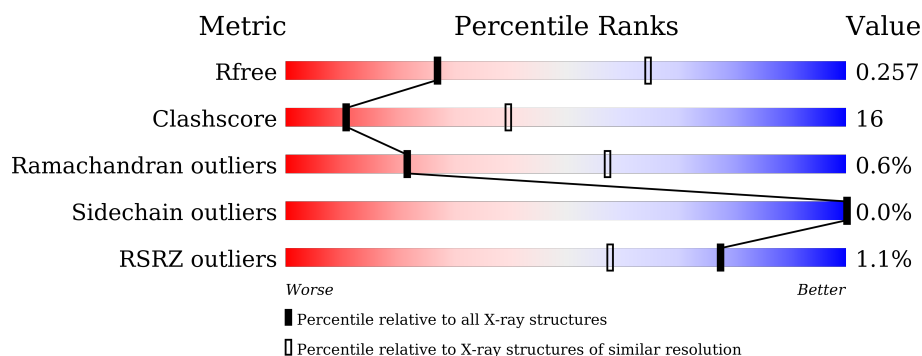
1 Overall quality at a glance

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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (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	<div> <div></div> <div>72%</div> <div>26%</div> <div>..</div> </div>
1	B	390	<div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div>
1	C	390	<div> <div></div> <div>69%</div> <div>28%</div> <div>..</div> </div>
1	D	390	<div> <div>2%</div> <div></div> <div>64%</div> <div>33%</div> <div>..</div> </div>
1	E	390	<div> <div></div> <div>69%</div> <div>28%</div> <div>..</div> </div>
1	F	390	<div> <div>2%</div> <div></div> <div>70%</div> <div>28%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	390	<div><div><div></div><div></div><div></div></div><div>2%61%22%16%</div><div></div></div>
1	H	390	<div><div><div></div><div></div><div></div></div><div>%64%33%..</div><div></div></div>
1	I	390	<div><div><div></div><div></div><div></div></div><div>69%29%..</div><div></div></div>
1	J	390	<div><div><div></div><div></div><div></div></div><div>4%64%33%..</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27964 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	384	Total	C	N	O	S	0	0	0
			2834	1783	486	551	14			
1	E	384	Total	C	N	O	S	0	0	0
			2834	1783	486	551	14			
1	G	329	Total	C	N	O	S	0	0	0
			2424	1526	413	473	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	384	Total	C	N	O	S	0	0	0
			2834	1783	486	551	14			

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Cl 1	0	0
3	I	1	Total 1	Cl 1	0	0

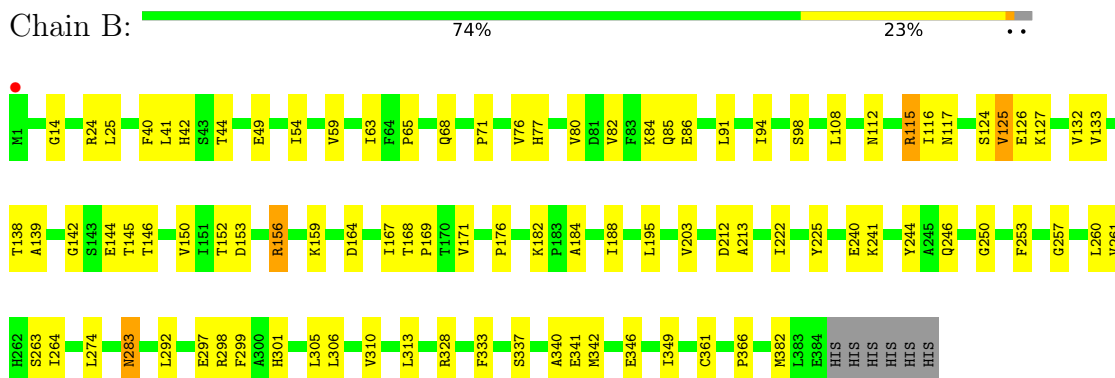
- Molecule 4 is water.

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

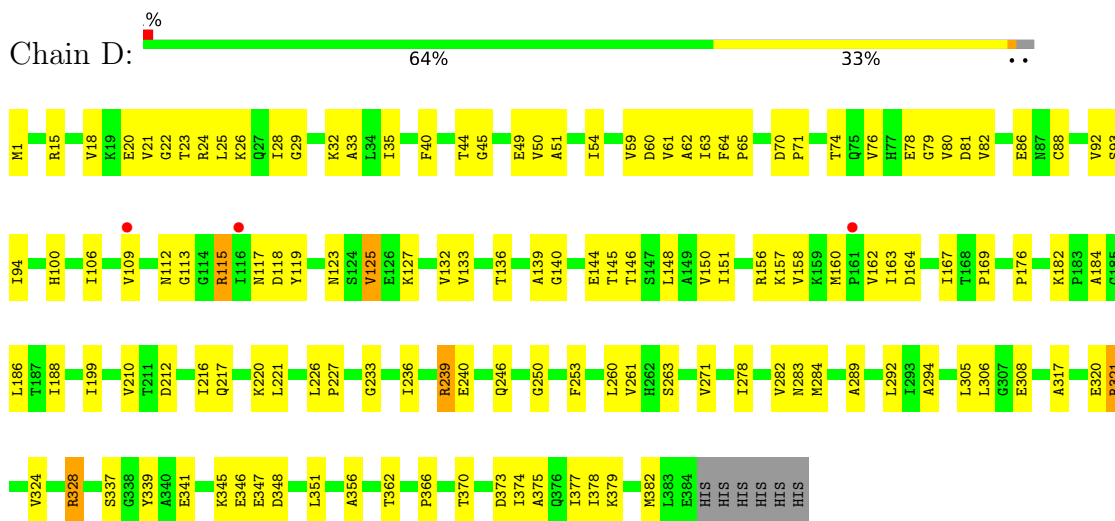
3 Residue-property plots

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.

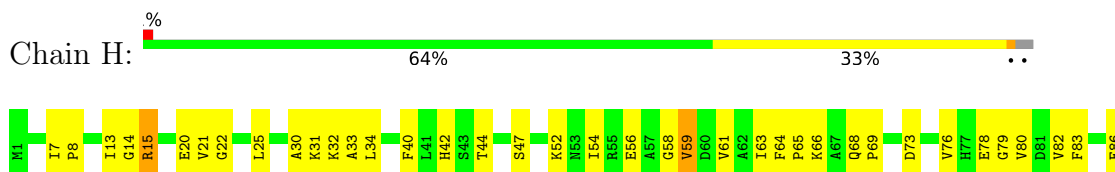
- Molecule 1: NAD(P)-dependent methanol dehydrogenase

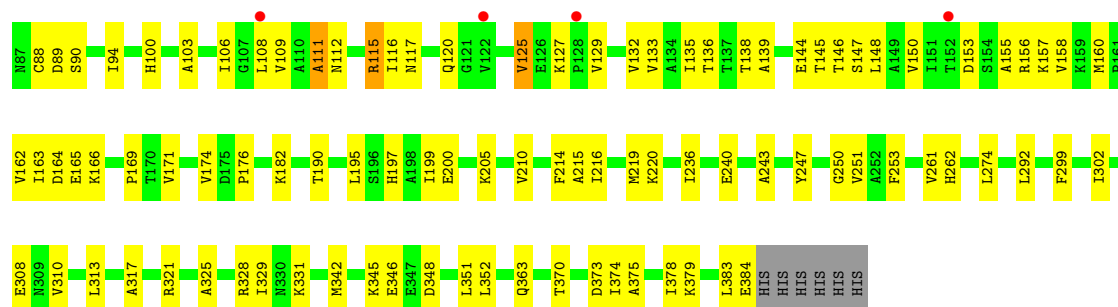


- Molecule 1: NAD(P)-dependent methanol dehydrogenase

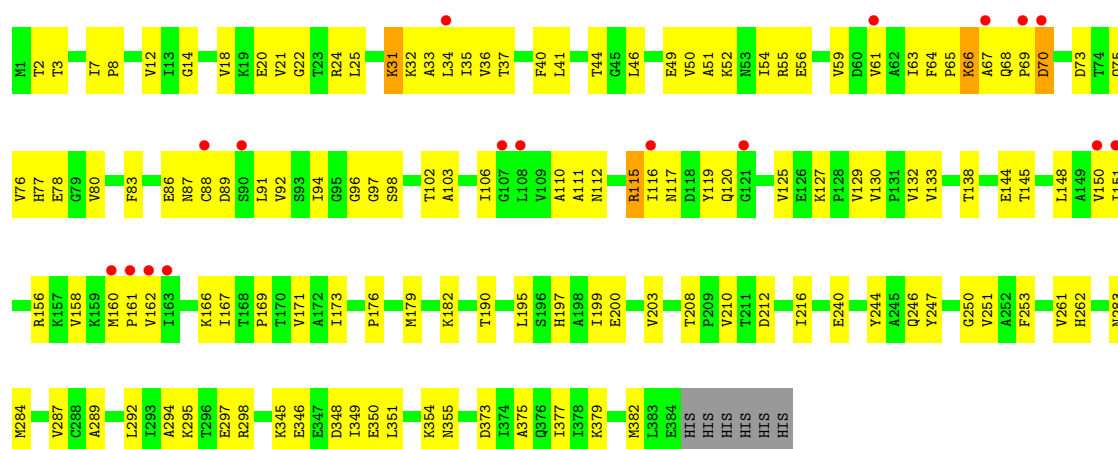


- Molecule 1: NAD(P)-dependent methanol dehydrogenase

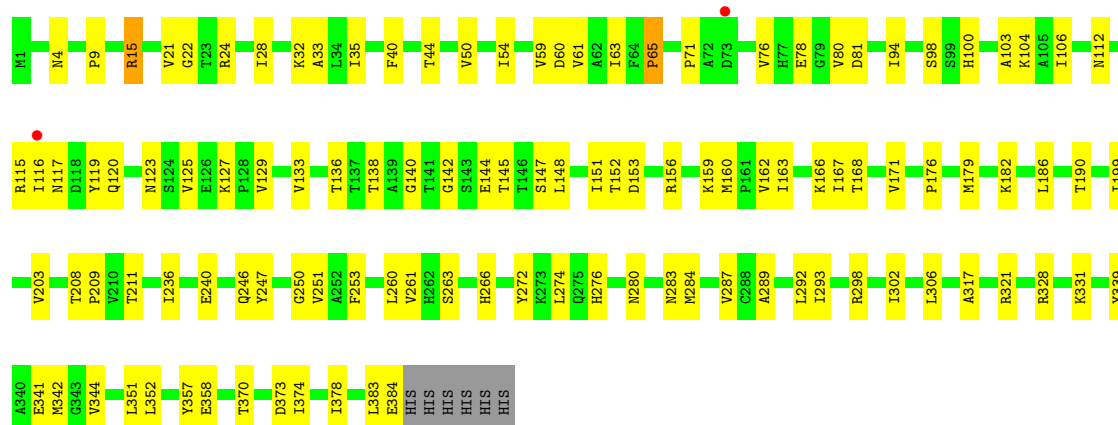




• Molecule 1: NAD(P)-dependent methanol dehydrogenase

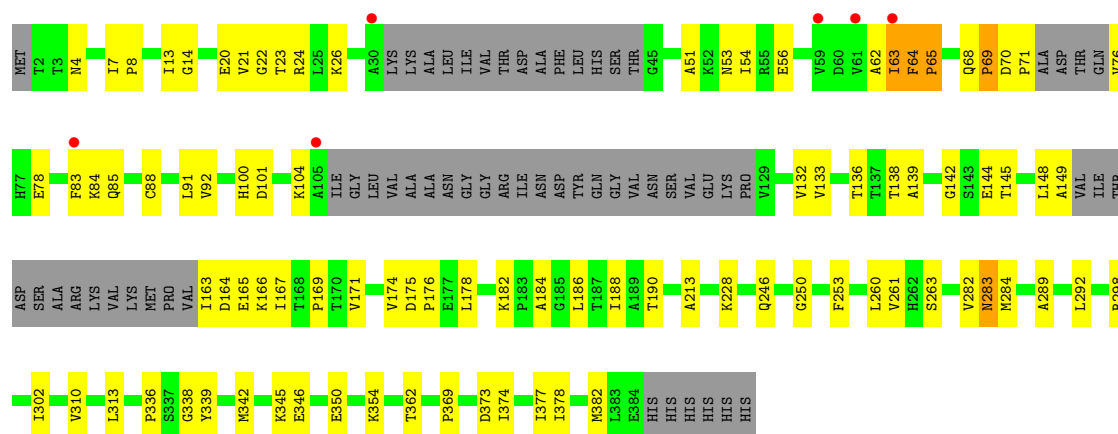


• Molecule 1: NAD(P)-dependent methanol dehydrogenase

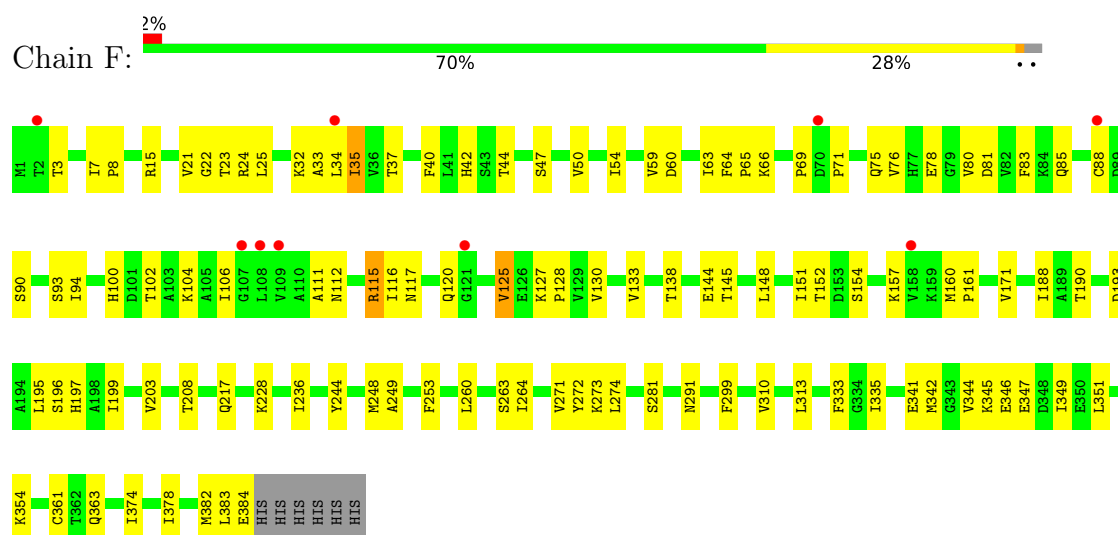


• Molecule 1: NAD(P)-dependent methanol dehydrogenase

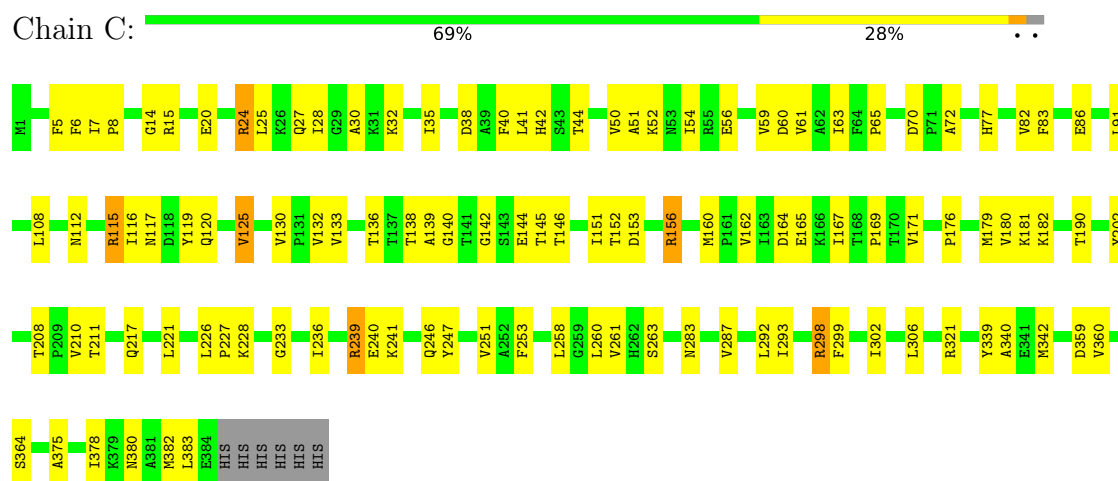




• Molecule 1: NAD(P)-dependent methanol dehydrogenase

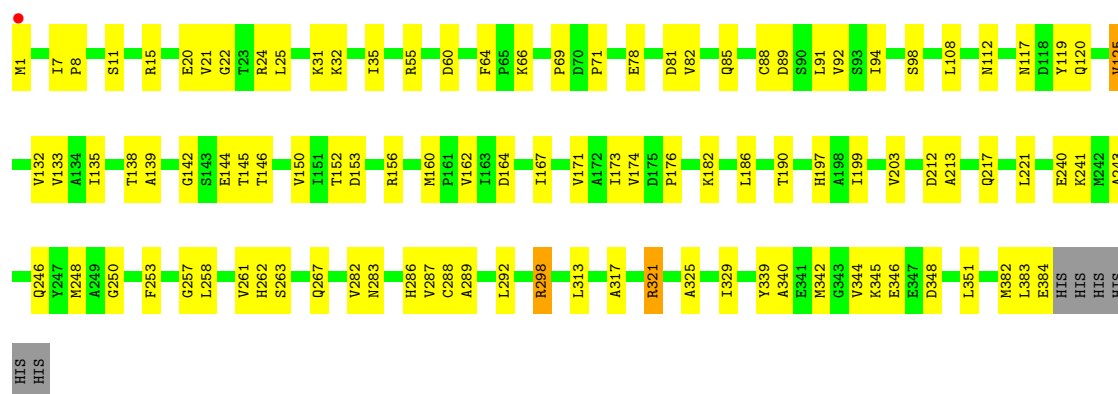


• Molecule 1: NAD(P)-dependent methanol dehydrogenase



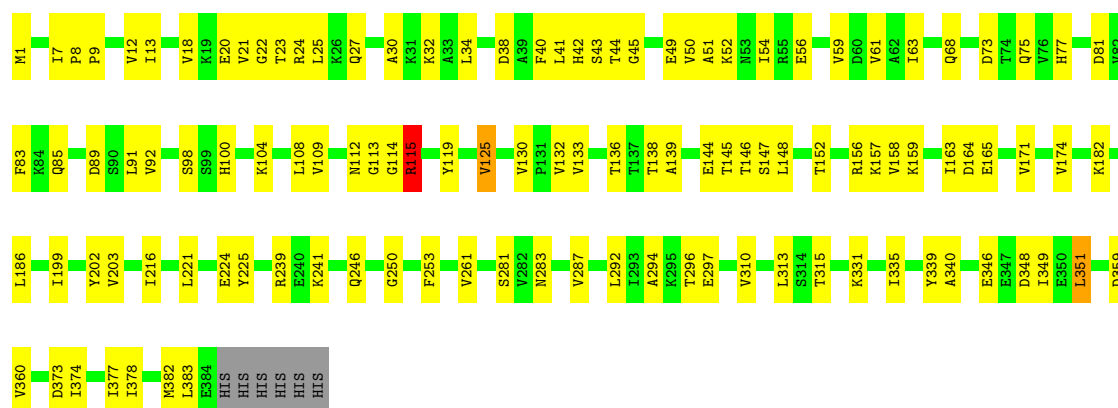
• Molecule 1: NAD(P)-dependent methanol dehydrogenase





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

Chain I: 69% 29% ..



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)	29.78 – 3.00 29.78 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.78-3.00) 95.4 (29.78-3.00)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.213 , 0.260 0.212 , 0.257	Depositor DCC
R_{free} test set	4737 reflections (4.95%)	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 , 58.3	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	27964	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.50	0/2877	0.78	2/3906 (0.1%)
1	B	0.53	1/2886 (0.0%)	0.84	1/3918 (0.0%)
1	C	0.51	0/2877	0.77	0/3906
1	D	0.50	0/2877	0.78	0/3906
1	E	0.57	2/2877 (0.1%)	0.84	2/3906 (0.1%)
1	F	0.49	0/2877	0.80	0/3906
1	G	0.55	1/2458 (0.0%)	0.84	1/3332 (0.0%)
1	H	0.48	0/2877	0.79	0/3906
1	I	0.55	0/2877	0.82	1/3906 (0.0%)
1	J	0.51	0/2877	0.82	2/3906 (0.1%)
All	All	0.52	4/28360 (0.0%)	0.81	9/38498 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	6
1	D	0	4
1	E	0	2
1	F	0	1
1	H	0	3
1	I	0	2
1	J	0	2
All	All	0	27

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	65	PRO	N-CD	8.72	1.59	1.47
1	E	65	PRO	CG-CD	-7.53	1.25	1.50
1	B	283	ASN	CB-CG	-5.64	1.38	1.52
1	G	283	ASN	CB-CG	-5.16	1.39	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	65	PRO	N-CD-CG	-14.91	80.84	103.20
1	I	351	LEU	CB-CG-CD2	-9.45	82.34	110.70
1	G	369	PRO	CA-N-CD	-8.03	100.76	112.00
1	E	65	PRO	N-CA-CB	-7.63	95.23	103.25
1	J	31	LYS	CB-CG-CD	6.33	125.87	111.30
1	J	70	ASP	CA-CB-CG	5.91	118.50	112.60
1	A	321	ARG	CA-CB-CG	-5.13	103.84	114.10
1	B	257	GLY	N-CA-C	5.06	117.21	111.85
1	A	257	GLY	N-CA-C	5.01	117.16	111.85

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ARG	Sidechain
1	A	298	ARG	Sidechain
1	A	55	ARG	Sidechain
1	B	115	ARG	Sidechain
1	B	156	ARG	Sidechain
1	B	24	ARG	Sidechain
1	B	328	ARG	Sidechain
1	C	115	ARG	Sidechain
1	C	156	ARG	Sidechain
1	C	239	ARG	Sidechain
1	C	24	ARG	Sidechain
1	C	298	ARG	Sidechain
1	C	321	ARG	Sidechain
1	D	115	ARG	Sidechain
1	D	239	ARG	Sidechain
1	D	321	ARG	Sidechain
1	D	328	ARG	Sidechain
1	E	15	ARG	Sidechain
1	E	156	ARG	Sidechain
1	F	115	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	H	115	ARG	Sidechain
1	H	15	ARG	Sidechain
1	H	328	ARG	Sidechain
1	I	115	ARG	Sidechain
1	I	239	ARG	Sidechain
1	J	115	ARG	Sidechain
1	J	156	ARG	Sidechain

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	82	0
1	B	2840	0	2885	76	0
1	C	2834	0	2879	86	0
1	D	2834	0	2879	113	0
1	E	2834	0	2879	94	0
1	F	2834	0	2879	79	1
1	G	2424	0	2443	86	1
1	H	2834	0	2879	116	0
1	I	2834	0	2879	89	0
1	J	2834	0	2879	128	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	E	1	0	0	0	0
3	I	1	0	0	0	0
4	A	2	0	0	0	0
4	B	4	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	3	0	0	0	0
4	I	1	0	0	0	0
All	All	27964	0	28360	923	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 16.

All (923) 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:H:348:ASP:O	1:H:351:LEU:HD23	1.17	1.34
1:G:148:LEU:HD22	1:G:163:ILE:CG2	1.59	1.29
1:H:348:ASP:O	1:H:351:LEU:CD2	1.87	1.21
1:D:113:GLY:O	1:D:115:ARG:NH2	1.75	1.18
1:B:142:GLY:HA2	1:B:246:GLN:NE2	1.59	1.18
1:E:142:GLY:HA2	1:E:246:GLN:HE21	1.09	1.17
1:E:142:GLY:HA2	1:E:246:GLN:NE2	1.60	1.16
1:G:68:GLN:HG3	1:G:69:PRO:HD3	1.26	1.11
1:H:250:GLY:HA2	1:H:253:PHE:CE2	1.87	1.09
1:G:148:LEU:CD2	1:G:163:ILE:HG23	1.80	1.09
1:J:117:ASN:HA	1:J:160:MET:HE1	1.34	1.08
1:A:142:GLY:HA2	1:A:246:GLN:NE2	1.69	1.07
1:B:142:GLY:CA	1:B:246:GLN:HE21	1.68	1.07
1:A:142:GLY:HA2	1:A:246:GLN:HE21	1.18	1.06
1:E:208:THR:HG22	1:E:211:THR:HG23	1.37	1.05
1:G:148:LEU:HD22	1:G:163:ILE:HG23	1.03	1.03
1:D:250:GLY:HA2	1:D:253:PHE:CE2	1.95	1.02
1:H:250:GLY:HA2	1:H:253:PHE:CD2	1.96	1.00
1:C:139:ALA:HA	1:C:246:GLN:OE1	1.63	0.99
1:E:142:GLY:CA	1:E:246:GLN:HE21	1.75	0.99
1:B:132:VAL:HG13	1:B:169:PRO:HA	1.43	0.98
1:B:142:GLY:HA2	1:B:246:GLN:HE21	0.81	0.97
1:G:68:GLN:HG3	1:G:69:PRO:CD	1.94	0.97
1:C:132:VAL:HG13	1:C:169:PRO:HA	1.46	0.95
1:B:115:ARG:HG3	1:B:117:ASN:OD1	1.69	0.93
1:E:176:PRO:HG3	1:E:240:GLU:HG3	1.50	0.91
1:A:142:GLY:CA	1:A:246:GLN:HE21	1.83	0.91
1:A:133:VAL:HG22	1:A:171:VAL:HB	1.52	0.91
1:J:32:LYS:NZ	1:J:86:GLU:O	2.05	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:77:HIS:HB2	1:J:115:ARG:HH22	1.35	0.89
1:E:383:LEU:HD12	1:E:384:GLU:HB3	1.55	0.89
1:B:132:VAL:CG1	1:B:169:PRO:HA	2.03	0.88
1:J:32:LYS:HB2	1:J:89:ASP:H	1.37	0.87
1:G:148:LEU:CD2	1:G:163:ILE:CG2	2.44	0.86
1:J:91:LEU:HD12	1:J:130:VAL:CG2	2.05	0.86
1:H:132:VAL:HG13	1:H:169:PRO:HA	1.56	0.86
1:H:63:ILE:HG22	1:H:65:PRO:HD3	1.57	0.86
1:C:133:VAL:HG22	1:C:171:VAL:HB	1.57	0.86
1:D:132:VAL:HG13	1:D:169:PRO:HA	1.58	0.85
1:D:63:ILE:HG22	1:D:65:PRO:HD3	1.58	0.85
1:J:111:ALA:HB1	1:J:127:LYS:HG3	1.57	0.85
1:D:148:LEU:HD13	1:D:163:ILE:HG13	1.59	0.85
1:J:117:ASN:HA	1:J:160:MET:CE	2.09	0.83
1:H:176:PRO:HG3	1:H:240:GLU:HG2	1.60	0.83
1:A:176:PRO:HG3	1:A:240:GLU:HG3	1.60	0.82
1:G:250:GLY:HA2	1:G:253:PHE:CD2	2.14	0.82
1:G:282:VAL:HG21	1:G:342:MET:HE1	1.61	0.82
1:H:146:THR:HG21	1:H:253:PHE:CZ	2.14	0.81
1:E:289:ALA:HA	1:E:292:LEU:HD13	1.61	0.81
1:J:25:LEU:HD23	1:J:54:ILE:HG23	1.62	0.80
1:B:250:GLY:HA2	1:B:253:PHE:CE2	2.17	0.80
1:A:289:ALA:HA	1:A:292:LEU:HD13	1.62	0.79
1:G:336:PRO:HB2	1:G:342:MET:HE2	1.63	0.79
1:D:146:THR:HG21	1:D:253:PHE:HZ	1.48	0.78
1:C:15:ARG:HG3	1:A:1:MET:HG3	1.64	0.78
1:I:25:LEU:HD23	1:I:59:VAL:HG11	1.66	0.78
1:F:133:VAL:HG22	1:F:171:VAL:HB	1.64	0.78
1:D:250:GLY:HA2	1:D:253:PHE:CD2	2.19	0.77
1:I:250:GLY:HA2	1:I:253:PHE:CD2	2.19	0.77
1:H:133:VAL:HG22	1:H:171:VAL:HB	1.67	0.77
1:B:144:GLU:CD	1:B:246:GLN:HE22	1.91	0.77
1:H:348:ASP:HB3	1:H:351:LEU:HD21	1.67	0.77
1:G:83:PHE:CZ	1:G:91:LEU:HD21	2.19	0.77
1:J:148:LEU:HD21	1:J:150:VAL:HG22	1.67	0.77
1:D:148:LEU:HD13	1:D:163:ILE:CG1	2.14	0.76
1:G:250:GLY:HA2	1:G:253:PHE:CE2	2.19	0.76
1:B:188:ILE:HD13	1:B:333:PHE:HB3	1.68	0.76
1:J:132:VAL:HG13	1:J:169:PRO:HA	1.67	0.75
1:A:171:VAL:CG1	1:A:173:ILE:HD11	2.17	0.75
1:D:351:LEU:HD12	1:D:351:LEU:H	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:CYS:O	1:A:292:LEU:CD1	2.33	0.75
1:E:383:LEU:HD12	1:E:384:GLU:CB	2.16	0.75
1:A:144:GLU:HG2	1:A:145:THR:HG23	1.69	0.75
1:F:76:VAL:O	1:F:80:VAL:HG23	1.87	0.75
1:D:148:LEU:HD12	1:D:162:VAL:O	1.86	0.74
1:F:54:ILE:HG22	1:F:59:VAL:HB	1.68	0.74
1:I:250:GLY:HA2	1:I:253:PHE:CE2	2.20	0.74
1:A:250:GLY:HA2	1:A:253:PHE:CE2	2.22	0.74
1:F:81:ASP:O	1:F:85:GLN:HG2	1.89	0.73
1:E:151:ILE:O	1:E:160:MET:HG2	1.88	0.73
1:D:148:LEU:CD1	1:D:163:ILE:HG13	2.18	0.72
1:G:213:ALA:HB2	1:F:217:GLN:HG3	1.71	0.72
1:B:144:GLU:OE2	1:B:246:GLN:NE2	2.20	0.72
1:D:184:ALA:O	1:D:188:ILE:HG13	1.90	0.72
1:J:73:ASP:OD2	1:J:116:ILE:CG2	2.38	0.72
1:I:25:LEU:HG	1:I:30:ALA:HB3	1.71	0.72
1:G:148:LEU:HD22	1:G:163:ILE:HG22	1.71	0.71
1:G:136:THR:HG22	1:G:138:THR:H	1.55	0.71
1:I:351:LEU:HD12	1:I:351:LEU:H	1.56	0.71
1:B:292:LEU:HD12	1:B:299:PHE:CD2	2.26	0.71
1:J:7:ILE:HD12	1:J:251:VAL:HG11	1.73	0.71
1:D:112:ASN:ND2	1:D:127:LYS:HB2	2.05	0.71
1:D:146:THR:HG21	1:D:253:PHE:CZ	2.25	0.70
1:H:144:GLU:HG2	1:H:145:THR:HG23	1.73	0.70
1:H:348:ASP:C	1:H:351:LEU:CD2	2.64	0.70
1:G:165:GLU:HG2	1:G:166:LYS:H	1.54	0.70
1:G:70:ASP:HA	1:G:76:VAL:HG12	1.72	0.70
1:G:175:ASP:HB3	1:G:178:LEU:HG	1.74	0.70
1:J:54:ILE:HG22	1:J:59:VAL:HB	1.74	0.69
1:J:68:GLN:HG3	1:J:69:PRO:O	1.91	0.69
1:C:51:ALA:HB1	1:C:61:VAL:HG21	1.74	0.69
1:J:295:LYS:HE3	1:J:298:ARG:HD3	1.75	0.69
1:A:339:TYR:HA	1:A:342:MET:HE3	1.74	0.69
1:B:139:ALA:H	1:B:182:LYS:NZ	1.89	0.69
1:D:370:THR:H	1:D:373:ASP:HB2	1.58	0.69
1:G:53:ASN:HA	1:G:56:GLU:HG3	1.72	0.69
1:J:25:LEU:CD2	1:J:54:ILE:HG23	2.23	0.69
1:J:250:GLY:HA2	1:J:253:PHE:CE2	2.27	0.69
1:H:34:LEU:HB2	1:H:88:CYS:SG	2.33	0.69
1:J:51:ALA:HB1	1:J:61:VAL:HG21	1.75	0.69
1:D:176:PRO:HG3	1:D:240:GLU:HG2	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:PRO:HD3	1:G:76:VAL:HA	1.76	0.68
1:C:139:ALA:CA	1:C:246:GLN:OE1	2.39	0.68
1:A:288:CYS:O	1:A:292:LEU:HD12	1.92	0.68
1:I:157:LYS:HE3	1:I:157:LYS:HA	1.76	0.68
1:F:144:GLU:HG2	1:F:145:THR:HG23	1.75	0.67
1:B:139:ALA:H	1:B:182:LYS:HZ2	1.43	0.67
1:J:345:LYS:NZ	1:J:348:ASP:HB2	2.09	0.67
1:H:274:LEU:HD13	1:H:342:MET:HE2	1.76	0.67
1:B:337:SER:HB2	1:B:341:GLU:OE2	1.93	0.67
1:H:139:ALA:H	1:H:182:LYS:HZ1	1.42	0.67
1:E:208:THR:CG2	1:E:211:THR:HG23	2.19	0.67
1:A:171:VAL:HG11	1:A:173:ILE:HD11	1.76	0.67
1:J:345:LYS:HZ1	1:J:348:ASP:HB2	1.58	0.67
1:E:136:THR:HG22	1:E:138:THR:H	1.58	0.67
1:E:144:GLU:OE2	1:E:246:GLN:NE2	2.23	0.66
1:D:32:LYS:HD3	1:D:60:ASP:HB3	1.78	0.66
1:E:144:GLU:CD	1:E:246:GLN:HE22	2.03	0.66
1:B:133:VAL:HG22	1:B:171:VAL:HB	1.78	0.66
1:E:120:GLN:HA	1:E:162:VAL:HG22	1.78	0.66
1:B:203:VAL:O	1:B:366:PRO:HG3	1.96	0.66
1:E:153:ASP:HB2	1:E:160:MET:HE2	1.78	0.66
1:F:35:ILE:HG23	1:F:94:ILE:HD13	1.78	0.66
1:J:77:HIS:HB2	1:J:115:ARG:NH2	2.10	0.65
1:H:94:ILE:HG12	1:H:135:ILE:HD12	1.79	0.65
1:E:147:SER:HB3	1:E:168:THR:OG1	1.96	0.65
1:G:68:GLN:CG	1:G:69:PRO:CD	2.74	0.65
1:H:32:LYS:HG2	1:H:88:CYS:HA	1.79	0.65
1:J:346:GLU:HA	1:J:349:ILE:HG13	1.78	0.65
1:E:129:VAL:HG22	1:E:166:LYS:HB3	1.77	0.65
1:A:250:GLY:HA2	1:A:253:PHE:CD2	2.32	0.65
1:D:217:GLN:HG2	4:D:501:HOH:O	1.96	0.65
1:H:13:ILE:HG23	1:H:174:VAL:HB	1.78	0.65
1:J:148:LEU:CD2	1:J:150:VAL:HG23	2.26	0.65
1:E:383:LEU:HD12	1:E:384:GLU:N	2.12	0.65
1:E:76:VAL:O	1:E:80:VAL:HG23	1.97	0.65
1:G:83:PHE:CE1	1:G:91:LEU:HD21	2.31	0.65
1:D:146:THR:CG2	1:D:253:PHE:CZ	2.79	0.65
1:C:54:ILE:HG22	1:C:59:VAL:HB	1.79	0.65
1:I:310:VAL:O	1:I:313:LEU:HB2	1.97	0.65
1:J:148:LEU:CD2	1:J:150:VAL:CG2	2.75	0.64
1:I:50:VAL:O	1:I:54:ILE:HG13	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:THR:HG21	1:H:253:PHE:HZ	1.59	0.64
1:H:346:GLU:H	1:H:346:GLU:CD	2.05	0.64
1:G:310:VAL:O	1:G:313:LEU:HB2	1.98	0.64
1:J:132:VAL:CG1	1:J:169:PRO:HA	2.28	0.64
1:H:15:ARG:HD2	1:H:236:ILE:HG12	1.79	0.64
1:E:182:LYS:HE3	1:E:186:LEU:HG	1.79	0.64
1:H:348:ASP:CA	1:H:351:LEU:CD2	2.76	0.64
1:A:282:VAL:HG21	1:A:342:MET:HE1	1.77	0.64
1:H:120:GLN:HG3	1:H:160:MET:HB3	1.79	0.64
1:J:148:LEU:HD21	1:J:150:VAL:CG2	2.28	0.64
1:A:351:LEU:HD12	1:A:351:LEU:H	1.62	0.64
1:B:164:ASP:O	1:B:167:ILE:HG12	1.97	0.64
1:C:221:LEU:HD22	1:C:241:LYS:HB3	1.78	0.64
1:I:144:GLU:HG2	1:I:145:THR:HG23	1.80	0.63
1:J:76:VAL:HG21	1:J:151:ILE:HG12	1.80	0.63
1:H:148:LEU:HD12	1:H:163:ILE:HD11	1.80	0.63
1:E:32:LYS:HD3	1:E:60:ASP:HB3	1.80	0.63
1:C:24:ARG:HA	1:C:27:GLN:HG3	1.79	0.63
1:B:108:LEU:HD11	1:B:125:VAL:HG21	1.81	0.63
1:H:40:PHE:O	1:H:44:THR:HG23	1.98	0.63
1:G:164:ASP:O	1:G:167:ILE:HG12	1.98	0.63
1:C:339:TYR:HB2	1:C:382:MET:HG2	1.80	0.63
1:G:70:ASP:CA	1:G:76:VAL:HG12	2.28	0.62
1:A:286:HIS:NE2	1:A:384:GLU:OE1	2.33	0.62
1:A:288:CYS:O	1:A:292:LEU:HD13	1.99	0.62
1:H:370:THR:H	1:H:373:ASP:HB2	1.63	0.62
1:C:117:ASN:ND2	1:C:153:ASP:OD1	2.32	0.62
1:J:12:VAL:HB	1:J:173:ILE:HD13	1.80	0.62
1:D:76:VAL:O	1:D:80:VAL:HG23	1.98	0.62
1:J:77:HIS:CB	1:J:115:ARG:HH22	2.11	0.62
1:C:50:VAL:O	1:C:54:ILE:HG13	1.99	0.62
1:C:132:VAL:CG1	1:C:169:PRO:HA	2.23	0.62
1:C:339:TYR:HA	1:C:342:MET:HE3	1.80	0.62
1:J:35:ILE:HG23	1:J:94:ILE:HD13	1.82	0.62
1:G:339:TYR:HA	1:G:342:MET:HE3	1.81	0.62
1:I:73:ASP:OD1	1:I:73:ASP:N	2.29	0.62
1:G:76:VAL:HG23	1:G:78:GLU:HG3	1.82	0.62
1:B:250:GLY:HA2	1:B:253:PHE:CD2	2.34	0.62
1:J:73:ASP:OD2	1:J:116:ILE:HG23	1.98	0.62
1:J:102:THR:O	1:J:106:ILE:HG13	1.99	0.62
1:C:116:ILE:HA	1:C:119:TYR:HD2	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:117:ASN:CA	1:J:160:MET:HE1	2.21	0.61
1:C:63:ILE:HG22	1:C:65:PRO:HD3	1.81	0.61
1:B:225:TYR:CZ	1:B:241:LYS:HD2	2.36	0.61
1:E:133:VAL:HG22	1:E:171:VAL:HB	1.82	0.61
1:D:250:GLY:HA2	1:D:253:PHE:HE2	1.61	0.61
1:D:347:GLU:HG3	1:D:348:ASP:OD1	2.01	0.61
1:C:42:HIS:CE1	1:C:63:ILE:HG21	2.34	0.61
1:I:40:PHE:O	1:I:43:SER:OG	2.18	0.61
1:J:77:HIS:CG	1:J:115:ARG:HH12	2.19	0.61
1:E:15:ARG:HD3	1:I:1:MET:SD	2.41	0.61
1:G:165:GLU:HG2	1:G:166:LYS:N	2.16	0.61
1:C:139:ALA:H	1:C:182:LYS:HZ3	1.49	0.61
1:H:132:VAL:CG1	1:H:169:PRO:HA	2.29	0.61
1:B:132:VAL:HG13	1:B:169:PRO:CA	2.25	0.61
1:J:91:LEU:HD12	1:J:130:VAL:HG21	1.83	0.61
1:F:93:SER:OG	1:F:100:HIS:HA	2.00	0.61
1:A:144:GLU:CD	1:A:246:GLN:HE22	2.08	0.61
1:D:151:ILE:O	1:D:160:MET:HG3	2.01	0.61
1:H:348:ASP:CB	1:H:351:LEU:HD21	2.30	0.61
1:G:83:PHE:CZ	1:G:91:LEU:HD11	2.36	0.61
1:E:142:GLY:N	1:E:246:GLN:HE21	1.98	0.60
1:F:71:PRO:O	1:F:152:THR:HG22	2.01	0.60
1:G:149:ALA:H	1:G:163:ILE:HD13	1.66	0.60
1:E:153:ASP:HB2	1:E:160:MET:CE	2.31	0.60
1:E:383:LEU:CD1	1:E:384:GLU:HB3	2.31	0.60
1:F:383:LEU:O	1:F:384:GLU:HB2	2.02	0.60
1:I:21:VAL:HG23	1:I:22:GLY:H	1.65	0.60
1:I:346:GLU:O	1:I:349:ILE:HG13	2.02	0.60
1:H:348:ASP:HA	1:H:351:LEU:HD22	1.83	0.60
1:J:250:GLY:HA2	1:J:253:PHE:CD2	2.37	0.60
1:C:151:ILE:O	1:C:160:MET:HG3	2.01	0.60
1:A:81:ASP:O	1:A:85:GLN:HG3	2.01	0.60
1:I:92:VAL:HG22	1:I:133:VAL:HB	1.83	0.60
1:B:212:ASP:CG	1:B:298:ARG:HH22	2.10	0.60
1:D:119:TYR:O	1:D:123:ASN:ND2	2.27	0.60
1:C:40:PHE:O	1:C:44:THR:HG23	2.01	0.60
1:H:139:ALA:H	1:H:182:LYS:NZ	1.99	0.60
1:E:112:ASN:OD1	1:E:127:LYS:HB2	2.01	0.60
1:C:32:LYS:HD2	1:C:60:ASP:HB3	1.84	0.59
1:B:71:PRO:O	1:B:152:THR:HG22	2.02	0.59
1:E:272:TYR:CE1	1:E:344:VAL:HG13	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:54:ILE:HG22	1:I:59:VAL:HB	1.84	0.59
1:D:132:VAL:CG1	1:D:169:PRO:HA	2.30	0.59
1:I:25:LEU:CD2	1:I:59:VAL:HG11	2.31	0.59
1:F:35:ILE:HD11	1:F:54:ILE:HD12	1.84	0.59
1:F:157:LYS:HE2	1:F:271:VAL:HA	1.84	0.59
1:H:31:LYS:N	1:H:89:ASP:OD2	2.32	0.59
1:H:200:GLU:CD	1:H:261:VAL:HB	2.27	0.59
1:H:210:VAL:HG23	1:J:244:TYR:HD1	1.68	0.59
1:E:63:ILE:HG22	1:E:65:PRO:HG3	1.84	0.59
1:E:272:TYR:CE2	1:E:344:VAL:HA	2.37	0.59
1:F:351:LEU:HD12	1:F:351:LEU:H	1.68	0.59
1:D:25:LEU:HD23	1:D:54:ILE:HG23	1.84	0.59
1:I:139:ALA:H	1:I:182:LYS:NZ	2.00	0.59
1:J:32:LYS:HD2	1:J:88:CYS:HA	1.84	0.58
1:C:340:ALA:HA	1:C:382:MET:HE3	1.84	0.58
1:H:64:PHE:CZ	1:H:79:GLY:HA2	2.38	0.58
1:J:64:PHE:CZ	1:J:66:LYS:HG2	2.38	0.58
1:C:139:ALA:H	1:C:182:LYS:NZ	2.02	0.58
1:F:363:GLN:N	1:F:363:GLN:OE1	2.37	0.58
1:B:115:ARG:HE	1:B:116:ILE:HG22	1.69	0.58
1:J:33:ALA:HB3	1:J:61:VAL:HG12	1.86	0.58
1:J:289:ALA:HA	1:J:292:LEU:HD13	1.86	0.58
1:I:77:HIS:HE1	1:I:115:ARG:H	1.50	0.58
1:C:7:ILE:HG13	1:C:8:PRO:HD2	1.86	0.58
1:H:146:THR:CG2	1:H:253:PHE:CZ	2.85	0.58
1:D:148:LEU:HD13	1:D:163:ILE:CD1	2.33	0.57
1:C:140:GLY:O	1:C:246:GLN:NE2	2.37	0.57
1:H:165:GLU:CD	1:J:24:ARG:HH22	2.12	0.57
1:H:250:GLY:CA	1:H:253:PHE:CE2	2.78	0.57
1:E:144:GLU:HG2	1:E:145:THR:HG23	1.87	0.57
1:C:283:ASN:ND2	1:C:287:VAL:HG23	2.20	0.57
1:I:108:LEU:HD11	1:I:125:VAL:HG21	1.85	0.57
1:B:146:THR:HG21	1:B:253:PHE:CZ	2.39	0.57
1:E:261:VAL:HA	1:E:283:ASN:OD1	2.03	0.57
1:G:70:ASP:C	1:G:76:VAL:HG12	2.29	0.57
1:A:142:GLY:N	1:A:246:GLN:HE21	2.01	0.57
1:I:52:LYS:O	1:I:56:GLU:HG3	2.05	0.57
1:H:117:ASN:HA	1:H:160:MET:HE1	1.86	0.57
1:H:112:ASN:OD1	1:H:125:VAL:HG13	2.05	0.57
1:I:148:LEU:HD12	1:I:163:ILE:HG13	1.87	0.57
1:D:112:ASN:HB3	1:D:119:TYR:OH	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:TYR:O	1:C:251:VAL:HG23	2.04	0.57
1:D:348:ASP:HA	1:D:351:LEU:HD13	1.86	0.57
1:J:37:THR:O	1:J:65:PRO:HA	2.04	0.57
1:J:246:GLN:HG3	1:J:247:TYR:N	2.19	0.57
1:H:78:GLU:O	1:H:82:VAL:HG23	2.05	0.56
1:H:348:ASP:HA	1:H:351:LEU:CD2	2.35	0.56
1:C:164:ASP:O	1:C:167:ILE:HG12	2.04	0.56
1:J:21:VAL:HG21	1:J:50:VAL:HG13	1.87	0.56
1:G:310:VAL:HA	1:G:313:LEU:HD12	1.86	0.56
1:B:77:HIS:HB2	1:B:115:ARG:HH12	1.69	0.56
1:D:21:VAL:HG13	1:D:22:GLY:H	1.70	0.56
1:J:129:VAL:CG2	1:J:166:LYS:HB3	2.35	0.56
1:J:7:ILE:HG13	1:J:8:PRO:HD2	1.87	0.56
1:C:120:GLN:HB2	1:C:160:MET:HE2	1.88	0.56
1:H:30:ALA:HB1	1:H:90:SER:HB3	1.87	0.56
1:A:146:THR:HG21	1:A:253:PHE:CZ	2.40	0.56
1:J:120:GLN:HA	1:J:161:PRO:O	2.06	0.56
1:G:144:GLU:HG2	1:G:145:THR:HG23	1.88	0.56
1:A:261:VAL:HG23	1:A:287:VAL:HG11	1.87	0.56
1:I:24:ARG:HA	1:I:27:GLN:OE1	2.06	0.56
1:I:133:VAL:HG22	1:I:171:VAL:HB	1.86	0.56
1:D:289:ALA:HA	1:D:292:LEU:HD13	1.87	0.56
1:J:96:GLY:O	1:J:98:SER:N	2.39	0.56
1:H:15:ARG:O	1:J:2:THR:OG1	2.23	0.56
1:F:15:ARG:HE	1:F:236:ILE:HG12	1.69	0.56
1:I:348:ASP:HA	1:I:351:LEU:HD13	1.88	0.56
1:H:21:VAL:HG13	1:H:22:GLY:H	1.71	0.56
1:J:129:VAL:HG22	1:J:166:LYS:HB3	1.87	0.56
1:G:76:VAL:CG2	1:G:78:GLU:HG3	2.36	0.56
1:I:156:ARG:HE	1:I:158:VAL:HG21	1.70	0.56
1:F:64:PHE:HZ	1:F:78:GLU:HG2	1.71	0.55
1:F:310:VAL:O	1:F:313:LEU:HB2	2.06	0.55
1:A:212:ASP:OD2	1:A:298:ARG:NH2	2.39	0.55
1:J:373:ASP:O	1:J:377:ILE:HG13	2.07	0.55
1:F:25:LEU:HD23	1:F:54:ILE:HG23	1.88	0.55
1:G:83:PHE:CZ	1:G:88:CYS:HB3	2.40	0.55
1:F:47:SER:HB2	1:F:63:ILE:HD13	1.88	0.55
1:F:102:THR:O	1:F:106:ILE:HD12	2.06	0.55
1:J:92:VAL:HG12	1:J:94:ILE:HD11	1.88	0.55
1:F:274:LEU:HD13	1:F:342:MET:HE2	1.88	0.55
1:I:109:VAL:HG13	1:I:114:GLY:HA2	1.86	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:138:THR:HG22	1:I:182:LYS:HD3	1.88	0.55
1:I:221:LEU:HD22	1:I:241:LYS:HB3	1.88	0.55
1:J:144:GLU:HG2	1:J:145:THR:HG23	1.89	0.55
1:A:108:LEU:HD11	1:A:125:VAL:HG21	1.89	0.55
1:I:42:HIS:CE1	1:I:63:ILE:HG21	2.42	0.55
1:D:64:PHE:CD1	1:D:82:VAL:HG21	2.42	0.55
1:D:374:ILE:O	1:D:378:ILE:HG13	2.06	0.55
1:F:80:VAL:HG22	1:F:106:ILE:HA	1.89	0.55
1:E:274:LEU:HD13	1:E:342:MET:HE2	1.89	0.54
1:G:64:PHE:N	1:G:65:PRO:HD3	2.22	0.54
1:D:233:GLY:HA3	1:D:239:ARG:HH21	1.73	0.54
1:J:64:PHE:HZ	1:J:78:GLU:HG2	1.72	0.54
1:I:182:LYS:HG2	1:I:186:LEU:HD23	1.89	0.54
1:B:85:GLN:HG3	1:B:86:GLU:HG2	1.88	0.54
1:H:76:VAL:O	1:H:80:VAL:HG23	2.08	0.54
1:I:112:ASN:OD1	1:I:125:VAL:HG13	2.07	0.54
1:D:112:ASN:HD21	1:D:125:VAL:HG13	1.73	0.54
1:J:346:GLU:HG3	1:J:349:ILE:HD12	1.90	0.54
1:F:138:THR:HB	1:F:190:THR:HG21	1.89	0.54
1:F:193:ASP:O	1:F:196:SER:HB3	2.07	0.54
1:G:132:VAL:HG13	1:G:169:PRO:HA	1.89	0.54
1:C:217:GLN:HG3	1:A:213:ALA:HB2	1.89	0.54
1:A:261:VAL:HA	1:A:283:ASN:OD1	2.08	0.54
1:B:77:HIS:CB	1:B:115:ARG:HH22	2.20	0.54
1:F:100:HIS:O	1:F:104:LYS:HG2	2.06	0.54
1:B:274:LEU:HD13	1:B:342:MET:HE2	1.88	0.54
1:F:374:ILE:O	1:F:378:ILE:HG13	2.08	0.54
1:D:32:LYS:NZ	1:D:86:GLU:OE2	2.40	0.54
1:H:148:LEU:HD21	1:H:150:VAL:HG23	1.88	0.54
1:G:148:LEU:CD2	1:G:163:ILE:HG22	2.33	0.54
1:I:139:ALA:H	1:I:182:LYS:HZ3	1.55	0.53
1:J:151:ILE:O	1:J:160:MET:HG2	2.09	0.53
1:H:138:THR:HB	1:H:190:THR:HG21	1.89	0.53
1:D:80:VAL:HG11	1:D:109:VAL:HG12	1.90	0.53
1:J:179:MET:O	1:J:182:LYS:HB2	2.08	0.53
1:A:78:GLU:O	1:A:82:VAL:HG23	2.08	0.53
1:D:199:ILE:HD13	1:D:284:MET:HE1	1.90	0.53
1:J:158:VAL:HG21	1:J:355:ASN:HD22	1.73	0.53
1:D:54:ILE:HG22	1:D:59:VAL:HB	1.91	0.53
1:D:148:LEU:HD13	1:D:163:ILE:HD11	1.90	0.53
1:E:40:PHE:O	1:E:44:THR:HG23	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HB	1:A:164:ASP:OD2	2.08	0.53
1:B:115:ARG:CG	1:B:117:ASN:OD1	2.51	0.53
1:B:260:LEU:HA	1:B:263:SER:HB2	1.90	0.53
1:B:261:VAL:HA	1:B:283:ASN:OD1	2.09	0.53
1:G:84:LYS:HD2	1:G:84:LYS:C	2.33	0.53
1:I:148:LEU:CD1	1:I:163:ILE:HG13	2.38	0.53
1:H:21:VAL:HG13	1:H:22:GLY:N	2.24	0.53
1:H:308:GLU:OE1	1:H:321:ARG:NH2	2.42	0.53
1:E:272:TYR:CZ	1:E:344:VAL:HA	2.44	0.53
1:H:384:GLU:OE2	1:H:384:GLU:HA	2.08	0.52
1:G:62:ALA:O	1:G:63:ILE:HG23	2.08	0.52
1:F:42:HIS:CD2	1:F:63:ILE:HG21	2.44	0.52
1:J:148:LEU:HD23	1:J:150:VAL:HG23	1.91	0.52
1:J:297:GLU:CD	1:J:297:GLU:H	2.17	0.52
1:J:375:ALA:O	1:J:379:LYS:HG3	2.09	0.52
1:A:346:GLU:H	1:A:346:GLU:CD	2.17	0.52
1:D:261:VAL:HG21	1:D:284:MET:HG2	1.91	0.52
1:I:136:THR:HG21	1:I:246:GLN:HE22	1.75	0.52
1:D:32:LYS:HE2	1:D:86:GLU:HG3	1.91	0.52
1:H:148:LEU:HD21	1:H:150:VAL:CG2	2.40	0.52
1:G:350:GLU:O	1:G:354:LYS:HG2	2.10	0.52
1:H:76:VAL:HG11	1:H:116:ILE:HD13	1.92	0.52
1:J:8:PRO:HG2	1:J:145:THR:HG22	1.91	0.52
1:E:120:GLN:NE2	1:E:160:MET:HB2	2.25	0.52
1:G:23:THR:O	1:G:26:LYS:HB3	2.10	0.52
1:G:83:PHE:HZ	1:G:91:LEU:HD21	1.71	0.52
1:J:103:ALA:HA	1:J:106:ILE:HD12	1.90	0.52
1:J:111:ALA:HB1	1:J:127:LYS:CG	2.34	0.52
1:G:84:LYS:HD2	1:G:85:GLN:N	2.25	0.52
1:A:171:VAL:CG1	1:A:173:ILE:CD1	2.88	0.52
1:E:261:VAL:HG23	1:E:287:VAL:HG11	1.92	0.52
1:C:236:ILE:O	1:C:240:GLU:HG3	2.09	0.52
1:B:77:HIS:HB2	1:B:115:ARG:NH1	2.25	0.52
1:D:24:ARG:O	1:D:28:ILE:HG13	2.10	0.52
1:D:139:ALA:H	1:D:182:LYS:NZ	2.08	0.52
1:H:14:GLY:HA3	1:J:2:THR:HA	1.92	0.52
1:H:348:ASP:CA	1:H:351:LEU:HD21	2.40	0.51
1:J:261:VAL:HA	1:J:283:ASN:OD1	2.09	0.51
1:H:210:VAL:HG23	1:J:244:TYR:CD1	2.45	0.51
1:H:250:GLY:HA2	1:H:253:PHE:HE2	1.64	0.51
1:G:148:LEU:HB3	1:G:163:ILE:HD12	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:ALA:HA	1:G:54:ILE:HD12	1.92	0.51
1:G:213:ALA:CB	1:F:217:GLN:HG3	2.39	0.51
1:J:35:ILE:HB	1:J:63:ILE:HD13	1.93	0.51
1:J:148:LEU:HD11	1:J:161:PRO:HB3	1.93	0.51
1:A:217:GLN:HG2	1:A:248:MET:HE1	1.93	0.51
1:I:38:ASP:OD1	1:I:41:LEU:HB2	2.10	0.51
1:H:42:HIS:HD2	1:H:65:PRO:HG3	1.76	0.51
1:J:21:VAL:HG23	1:J:22:GLY:H	1.75	0.51
1:J:46:LEU:HA	1:J:49:GLU:HG2	1.93	0.51
1:B:124:SER:OG	1:B:125:VAL:N	2.43	0.51
1:J:91:LEU:CD1	1:J:130:VAL:CG2	2.86	0.51
1:E:152:THR:HG23	1:E:159:LYS:HA	1.93	0.51
1:J:80:VAL:HG22	1:J:106:ILE:HA	1.92	0.51
1:A:286:HIS:CE1	1:A:384:GLU:OE1	2.64	0.51
1:A:317:ALA:O	1:A:321:ARG:HG2	2.10	0.51
1:H:199:ILE:HG23	1:H:302:ILE:HD13	1.93	0.50
1:C:112:ASN:OD1	1:C:125:VAL:HG13	2.11	0.50
1:D:32:LYS:HG3	1:D:88:CYS:SG	2.51	0.50
1:E:208:THR:HG23	1:E:211:THR:H	1.76	0.50
1:F:50:VAL:O	1:F:54:ILE:HG13	2.11	0.50
1:I:147:SER:HB3	1:I:164:ASP:O	2.11	0.50
1:B:54:ILE:HG23	1:B:59:VAL:HB	1.93	0.50
1:J:195:LEU:O	1:J:199:ILE:HG13	2.11	0.50
1:E:261:VAL:HG21	1:E:284:MET:HG3	1.92	0.50
1:G:350:GLU:HG3	1:G:354:LYS:HE2	1.94	0.50
1:F:33:ALA:HA	1:F:90:SER:O	2.12	0.50
1:F:120:GLN:CD	1:F:160:MET:HB3	2.37	0.50
1:C:139:ALA:C	1:C:246:GLN:OE1	2.55	0.50
1:D:35:ILE:N	1:D:62:ALA:O	2.45	0.50
1:H:73:ASP:HB3	1:H:116:ILE:HG21	1.94	0.50
1:J:351:LEU:H	1:J:351:LEU:HD12	1.77	0.50
1:E:24:ARG:NH1	1:I:165:GLU:OE2	2.42	0.50
1:F:112:ASN:OD1	1:F:125:VAL:HG13	2.12	0.50
1:F:345:LYS:NZ	1:F:347:GLU:HB2	2.27	0.50
1:A:64:PHE:CZ	1:A:66:LYS:HB2	2.47	0.50
1:D:261:VAL:HA	1:D:283:ASN:OD1	2.11	0.50
1:G:101:ASP:O	1:G:104:LYS:HB2	2.12	0.50
1:A:71:PRO:O	1:A:152:THR:HG22	2.12	0.50
1:F:64:PHE:CE2	1:F:66:LYS:HB2	2.47	0.50
1:B:195:LEU:HD13	1:B:222:ILE:HG21	1.94	0.50
1:C:292:LEU:HD12	1:C:299:PHE:CG	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:ARG:HD2	1:H:236:ILE:CG1	2.40	0.50
1:J:34:LEU:HG	1:J:36:VAL:HG22	1.93	0.50
1:C:77:HIS:NE2	1:C:115:ARG:HA	2.26	0.50
1:B:225:TYR:CE1	1:B:241:LYS:HD2	2.47	0.50
1:D:306:LEU:O	1:D:328:ARG:NH2	2.42	0.50
1:A:94:ILE:HG12	1:A:135:ILE:CD1	2.42	0.50
1:J:176:PRO:HG3	1:J:240:GLU:HG3	1.94	0.49
1:C:138:THR:HA	1:C:182:LYS:HD2	1.94	0.49
1:I:7:ILE:HG13	1:I:8:PRO:HD2	1.94	0.49
1:I:13:ILE:HG23	1:I:174:VAL:HB	1.92	0.49
1:C:116:ILE:HD11	1:C:162:VAL:HG11	1.94	0.49
1:C:144:GLU:HG2	1:C:145:THR:HG23	1.94	0.49
1:D:378:ILE:O	1:D:382:MET:HG2	2.11	0.49
1:E:115:ARG:HG2	1:E:117:ASN:H	1.77	0.49
1:C:25:LEU:HG	1:C:30:ALA:HB3	1.95	0.49
1:C:156:ARG:HH22	1:C:160:MET:HE3	1.77	0.49
1:C:208:THR:HG23	1:C:211:THR:H	1.77	0.49
1:D:233:GLY:CA	1:D:239:ARG:HH21	2.25	0.49
1:H:7:ILE:HG13	1:H:8:PRO:HD2	1.94	0.49
1:H:25:LEU:HD23	1:H:54:ILE:HG23	1.92	0.49
1:H:351:LEU:HD23	1:H:352:LEU:H	1.76	0.49
1:J:3:THR:HG21	1:J:208:THR:HG21	1.94	0.49
1:E:33:ALA:O	1:E:61:VAL:HA	2.12	0.49
1:G:14:GLY:O	1:G:176:PRO:HD2	2.13	0.49
1:G:261:VAL:HG21	1:G:284:MET:HG3	1.95	0.49
1:I:202:TYR:CE1	1:I:216:ILE:HD11	2.47	0.49
1:B:244:TYR:HD1	1:D:210:VAL:HG23	1.77	0.49
1:H:216:ILE:HG22	1:H:220:LYS:HD2	1.95	0.49
1:J:21:VAL:HG23	1:J:22:GLY:N	2.28	0.49
1:J:200:GLU:CD	1:J:261:VAL:HB	2.37	0.49
1:F:7:ILE:HG13	1:F:8:PRO:HD2	1.93	0.49
1:C:298:ARG:O	1:C:302:ILE:HG13	2.13	0.49
1:H:80:VAL:HG11	1:H:109:VAL:HB	1.94	0.49
1:E:50:VAL:HG21	1:E:94:ILE:HD13	1.95	0.49
1:B:80:VAL:O	1:B:84:LYS:HG2	2.13	0.49
1:B:340:ALA:HB2	1:B:382:MET:HE3	1.94	0.49
1:D:151:ILE:H	1:D:151:ILE:HD12	1.78	0.49
1:D:375:ALA:O	1:D:379:LYS:HG3	2.12	0.49
1:I:45:GLY:O	1:I:49:GLU:HG3	2.13	0.49
1:I:296:THR:HG22	1:I:315:THR:HG22	1.95	0.49
1:D:93:SER:OG	1:D:100:HIS:HA	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:VAL:HG22	1:E:106:ILE:HA	1.95	0.49
1:A:153:ASP:OD2	1:A:156:ARG:HB2	2.13	0.49
1:B:260:LEU:O	1:B:264:ILE:HD12	2.13	0.48
1:C:6:PHE:CE2	1:C:165:GLU:HB2	2.48	0.48
1:C:217:GLN:HG3	1:A:213:ALA:CB	2.42	0.48
1:A:21:VAL:HG13	1:A:22:GLY:H	1.77	0.48
1:A:221:LEU:HD22	1:A:241:LYS:HB3	1.95	0.48
1:D:136:THR:HG21	1:D:246:GLN:HE22	1.78	0.48
1:J:40:PHE:O	1:J:44:THR:HG23	2.13	0.48
1:E:63:ILE:HG22	1:E:65:PRO:CG	2.43	0.48
1:C:142:GLY:O	1:C:146:THR:HG23	2.13	0.48
1:B:152:THR:HA	1:B:159:LYS:HA	1.95	0.48
1:D:278:ILE:O	1:D:282:VAL:HG23	2.13	0.48
1:D:283:ASN:HB2	1:D:339:TYR:OH	2.12	0.48
1:G:7:ILE:HG13	1:G:8:PRO:HD2	1.96	0.48
1:F:35:ILE:HD11	1:F:54:ILE:CD1	2.44	0.48
1:B:76:VAL:O	1:B:80:VAL:HG23	2.14	0.48
1:D:112:ASN:HD21	1:D:127:LYS:HB2	1.78	0.48
1:H:58:GLY:O	1:H:59:VAL:HB	2.12	0.48
1:H:117:ASN:OD1	1:H:160:MET:SD	2.72	0.48
1:E:50:VAL:HG12	1:E:54:ILE:HD11	1.95	0.48
1:F:76:VAL:HG21	1:F:151:ILE:HG12	1.94	0.48
1:I:32:LYS:O	1:I:89:ASP:OD1	2.32	0.48
1:I:261:VAL:HG23	1:I:287:VAL:HG11	1.94	0.48
1:B:153:ASP:OD2	1:B:156:ARG:NE	2.43	0.48
1:J:148:LEU:HD11	1:J:161:PRO:CB	2.44	0.48
1:F:111:ALA:HB1	1:F:127:LYS:HD2	1.95	0.48
1:F:151:ILE:O	1:F:160:MET:N	2.47	0.48
1:C:38:ASP:OD1	1:C:41:LEU:HB2	2.13	0.48
1:D:18:VAL:O	1:D:21:VAL:HG12	2.14	0.48
1:D:345:LYS:HB3	1:D:347:GLU:HG2	1.96	0.48
1:J:133:VAL:HG22	1:J:171:VAL:HB	1.96	0.48
1:B:80:VAL:HG12	1:B:84:LYS:HZ2	1.78	0.48
1:B:126:GLU:HG3	1:B:127:LYS:HE2	1.96	0.48
1:H:33:ALA:O	1:H:61:VAL:HA	2.14	0.47
1:J:18:VAL:O	1:J:21:VAL:HG22	2.14	0.47
1:E:28:ILE:HD12	1:E:28:ILE:HG23	1.59	0.47
1:A:283:ASN:HD21	1:A:287:VAL:HG23	1.78	0.47
1:I:21:VAL:HG23	1:I:22:GLY:N	2.28	0.47
1:D:212:ASP:O	1:D:216:ILE:HD12	2.14	0.47
1:B:42:HIS:CE1	1:B:63:ILE:HG21	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:HIS:CE1	1:B:305:LEU:HD11	2.49	0.47
1:H:129:VAL:HG22	1:H:166:LYS:HE3	1.96	0.47
1:H:214:PHE:CE1	1:J:210:VAL:HG13	2.50	0.47
1:J:31:LYS:C	1:J:59:VAL:HG13	2.39	0.47
1:J:182:LYS:NZ	1:J:190:THR:OG1	2.37	0.47
1:F:127:LYS:HD3	1:F:128:PRO:HD2	1.96	0.47
1:C:83:PHE:CZ	1:C:130:VAL:HG21	2.49	0.47
1:I:351:LEU:H	1:I:351:LEU:CD1	2.25	0.47
1:H:31:LYS:O	1:H:59:VAL:HA	2.15	0.47
1:H:73:ASP:HA	1:H:76:VAL:HB	1.96	0.47
1:H:108:LEU:HD11	1:H:125:VAL:HG21	1.96	0.47
1:H:153:ASP:HB2	1:H:160:MET:SD	2.54	0.47
1:E:138:THR:C	1:E:179:MET:HE2	2.40	0.47
1:G:14:GLY:C	1:G:176:PRO:HD2	2.40	0.47
1:H:42:HIS:HA	1:H:47:SER:OG	2.13	0.47
1:E:21:VAL:HG13	1:E:22:GLY:H	1.80	0.47
1:E:260:LEU:HA	1:E:263:SER:HB2	1.95	0.47
1:C:20:GLU:HG3	1:C:24:ARG:HG3	1.95	0.47
1:A:20:GLU:O	1:A:24:ARG:HG3	2.14	0.47
1:A:150:VAL:HA	1:A:160:MET:O	2.14	0.47
1:A:199:ILE:O	1:A:203:VAL:HG22	2.13	0.47
1:B:77:HIS:HB3	1:B:115:ARG:HH22	1.80	0.47
1:H:195:LEU:O	1:H:199:ILE:HG13	2.15	0.47
1:G:374:ILE:O	1:G:378:ILE:HG13	2.15	0.47
1:F:228:LYS:NZ	1:C:293:ILE:O	2.47	0.47
1:C:52:LYS:O	1:C:56:GLU:HG3	2.14	0.47
1:B:184:ALA:O	1:B:188:ILE:HG13	2.14	0.47
1:H:157:LYS:N	1:H:157:LYS:HD2	2.29	0.47
1:E:208:THR:HG22	1:E:211:THR:CG2	2.26	0.47
1:E:370:THR:H	1:E:373:ASP:HB2	1.80	0.47
1:I:340:ALA:HB2	1:I:382:MET:HE3	1.95	0.47
1:D:146:THR:HG22	1:D:253:PHE:CZ	2.50	0.47
1:H:310:VAL:HA	1:H:313:LEU:HD12	1.97	0.47
1:F:195:LEU:O	1:F:199:ILE:HG13	2.15	0.47
1:I:374:ILE:O	1:I:378:ILE:HG13	2.14	0.47
1:B:310:VAL:O	1:B:313:LEU:HB2	2.16	0.46
1:D:51:ALA:HB1	1:D:61:VAL:HG21	1.96	0.46
1:D:118:ASP:OD1	1:D:118:ASP:N	2.48	0.46
1:H:214:PHE:CZ	1:J:210:VAL:HG13	2.50	0.46
1:F:34:LEU:HB2	1:F:88:CYS:SG	2.54	0.46
1:C:180:VAL:HG12	1:C:181:LYS:HD2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ASN:CG	1:B:127:LYS:HB2	2.40	0.46
1:H:197:HIS:CD2	1:H:262:HIS:CE1	3.03	0.46
1:H:331:LYS:HB3	1:H:331:LYS:HE2	1.63	0.46
1:E:140:GLY:O	1:E:142:GLY:N	2.45	0.46
1:F:21:VAL:HG13	1:F:22:GLY:N	2.29	0.46
1:C:179:MET:HB3	1:C:182:LYS:HD3	1.98	0.46
1:C:283:ASN:HD21	1:C:287:VAL:HG23	1.80	0.46
1:A:325:ALA:O	1:A:329:ILE:HD12	2.14	0.46
1:G:83:PHE:CZ	1:G:91:LEU:CD2	2.96	0.46
1:G:133:VAL:HG22	1:G:171:VAL:HB	1.98	0.46
1:F:50:VAL:HG12	1:F:54:ILE:HD11	1.97	0.46
1:I:77:HIS:CE1	1:I:115:ARG:HA	2.50	0.46
1:I:199:ILE:O	1:I:203:VAL:HG22	2.16	0.46
1:D:317:ALA:O	1:D:321:ARG:HG2	2.15	0.46
1:J:32:LYS:CD	1:J:88:CYS:HA	2.45	0.46
1:E:100:HIS:O	1:E:104:LYS:HG3	2.15	0.46
1:E:328:ARG:HA	1:E:331:LYS:HE3	1.97	0.46
1:B:40:PHE:O	1:B:44:THR:HG23	2.16	0.46
1:H:325:ALA:O	1:H:329:ILE:HG13	2.16	0.46
1:G:71:PRO:HB3	1:G:76:VAL:HB	1.97	0.46
1:C:14:GLY:C	1:C:176:PRO:HD2	2.41	0.46
1:I:83:PHE:CZ	1:I:130:VAL:HG11	2.50	0.46
1:I:152:THR:HA	1:I:159:LYS:HA	1.96	0.46
1:B:41:LEU:HD13	1:B:94:ILE:O	2.16	0.46
1:H:64:PHE:CE2	1:H:66:LYS:HB2	2.51	0.46
1:J:51:ALA:O	1:J:55:ARG:HG3	2.16	0.46
1:G:13:ILE:HG23	1:G:174:VAL:HB	1.97	0.46
1:F:188:ILE:HD13	1:F:333:PHE:HB3	1.98	0.46
1:C:359:ASP:OD1	1:C:360:VAL:N	2.48	0.46
1:A:35:ILE:HA	1:A:92:VAL:O	2.15	0.46
1:B:25:LEU:HD12	1:B:25:LEU:HA	1.73	0.46
1:D:25:LEU:HD23	1:D:54:ILE:CG2	2.46	0.46
1:H:348:ASP:O	1:H:351:LEU:HD21	2.02	0.46
1:I:25:LEU:HD23	1:I:54:ILE:CG2	2.46	0.46
1:D:21:VAL:HG13	1:D:22:GLY:N	2.31	0.46
1:D:157:LYS:HB3	1:D:271:VAL:HG22	1.98	0.46
1:G:289:ALA:HA	1:G:292:LEU:HD13	1.98	0.46
1:F:21:VAL:HG13	1:F:22:GLY:H	1.80	0.46
1:I:77:HIS:HE1	1:I:115:ARG:N	2.14	0.46
1:D:182:LYS:HG2	1:D:186:LEU:HD23	1.98	0.46
1:A:282:VAL:HG21	1:A:342:MET:CE	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:GLU:O	1:D:324:VAL:HG23	2.16	0.45
1:E:148:LEU:HD13	1:E:163:ILE:HG13	1.97	0.45
1:E:298:ARG:O	1:E:302:ILE:HG13	2.15	0.45
1:E:342:MET:HE2	1:E:342:MET:HB3	1.84	0.45
1:F:37:THR:O	1:F:65:PRO:HA	2.15	0.45
1:C:233:GLY:CA	1:C:239:ARG:HH21	2.29	0.45
1:I:51:ALA:HB1	1:I:61:VAL:HG21	1.97	0.45
1:D:32:LYS:NZ	1:D:86:GLU:HG3	2.31	0.45
1:D:80:VAL:HG22	1:D:106:ILE:HA	1.98	0.45
1:E:152:THR:HA	1:E:159:LYS:HA	1.98	0.45
1:E:272:TYR:HE1	1:E:352:LEU:HD11	1.82	0.45
1:G:148:LEU:HA	1:G:163:ILE:HA	1.98	0.45
1:F:260:LEU:HD21	1:F:374:ILE:HG12	1.98	0.45
1:I:331:LYS:HB3	1:I:331:LYS:HE3	1.68	0.45
1:H:292:LEU:HD12	1:H:299:PHE:CD2	2.52	0.45
1:E:351:LEU:H	1:E:351:LEU:HD12	1.81	0.45
1:A:94:ILE:HG12	1:A:135:ILE:HD12	1.97	0.45
1:A:339:TYR:HB2	1:A:382:MET:HA	1.99	0.45
1:B:346:GLU:O	1:B:349:ILE:HG13	2.16	0.45
1:D:308:GLU:OE2	1:D:321:ARG:NH2	2.50	0.45
1:E:15:ARG:HD2	1:E:236:ILE:CG1	2.47	0.45
1:E:116:ILE:HD11	1:E:162:VAL:HG11	1.99	0.45
1:G:100:HIS:O	1:G:104:LYS:HG2	2.16	0.45
1:C:83:PHE:CE1	1:C:91:LEU:HG	2.51	0.45
1:J:261:VAL:HG21	1:J:284:MET:HG3	1.98	0.45
1:E:4:ASN:OD1	1:I:12:VAL:HG22	2.16	0.45
1:J:31:LYS:C	1:J:31:LYS:HD3	2.42	0.45
1:E:250:GLY:HA2	1:E:253:PHE:CE2	2.51	0.45
1:C:28:ILE:HD11	1:C:171:VAL:CG2	2.46	0.45
1:H:52:LYS:HE3	1:H:56:GLU:CD	2.41	0.45
1:E:140:GLY:N	1:E:246:GLN:HG3	2.32	0.45
1:E:357:TYR:HB3	1:E:358:GLU:OE1	2.17	0.45
1:I:83:PHE:HZ	1:I:130:VAL:HG11	1.82	0.45
1:D:144:GLU:HG2	1:D:145:THR:HG23	1.97	0.45
1:C:380:ASN:O	1:C:383:LEU:HB2	2.17	0.45
1:J:69:PRO:O	1:J:70:ASP:C	2.60	0.45
1:E:9:PRO:HB3	1:I:9:PRO:HD3	1.99	0.45
1:G:101:ASP:OD2	1:G:149:ALA:HA	2.17	0.45
1:G:345:LYS:HB2	1:G:345:LYS:HE3	1.74	0.45
1:F:32:LYS:HD3	1:F:60:ASP:HB3	1.99	0.45
1:A:69:PRO:HA	1:A:98:SER:OG	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:LYS:O	1:D:29:GLY:N	2.48	0.45
1:J:14:GLY:C	1:J:176:PRO:HD2	2.42	0.45
1:A:117:ASN:HA	1:A:160:MET:HE1	1.98	0.45
1:D:260:LEU:HA	1:D:263:SER:HB2	1.99	0.44
1:J:33:ALA:O	1:J:61:VAL:HA	2.16	0.44
1:J:83:PHE:CZ	1:J:88:CYS:HB2	2.52	0.44
1:E:138:THR:HB	1:E:190:THR:HG21	1.99	0.44
1:E:199:ILE:HD11	1:E:306:LEU:HD11	2.00	0.44
1:G:165:GLU:O	1:G:166:LYS:HB2	2.17	0.44
1:A:186:LEU:O	1:A:190:THR:HG23	2.16	0.44
1:I:156:ARG:HE	1:I:158:VAL:CG2	2.29	0.44
1:D:79:GLY:HA2	1:D:82:VAL:HG22	1.98	0.44
1:E:71:PRO:HG3	1:E:98:SER:HA	1.99	0.44
1:F:75:GLN:HA	1:F:78:GLU:HB3	1.99	0.44
1:B:71:PRO:HG2	1:B:150:VAL:O	2.18	0.44
1:B:91:LEU:O	1:B:132:VAL:HA	2.17	0.44
1:D:15:ARG:HH11	1:D:236:ILE:HG21	1.83	0.44
1:D:32:LYS:CE	1:D:86:GLU:HG3	2.47	0.44
1:D:74:THR:O	1:D:78:GLU:HG3	2.17	0.44
1:D:356:ALA:O	1:D:362:THR:HG21	2.17	0.44
1:H:34:LEU:HD22	1:H:83:PHE:HD1	1.82	0.44
1:I:112:ASN:CG	1:I:125:VAL:HG13	2.42	0.44
1:D:139:ALA:H	1:D:182:LYS:HZ2	1.64	0.44
1:D:337:SER:HB2	1:D:341:GLU:OE2	2.17	0.44
1:H:64:PHE:CZ	1:H:79:GLY:CA	3.00	0.44
1:H:215:ALA:O	1:H:219:MET:HG3	2.17	0.44
1:C:72:ALA:HA	1:C:152:THR:HG22	2.00	0.44
1:A:339:TYR:HB3	1:A:344:VAL:HG21	2.00	0.44
1:I:136:THR:HG22	1:I:138:THR:H	1.82	0.44
1:B:213:ALA:HB2	1:D:217:GLN:HG3	2.00	0.44
1:D:164:ASP:O	1:D:167:ILE:HG12	2.17	0.44
1:D:370:THR:N	1:D:373:ASP:HB2	2.29	0.44
1:H:30:ALA:HB1	1:H:90:SER:CB	2.48	0.44
1:H:345:LYS:HB3	1:H:345:LYS:HE2	1.80	0.44
1:J:25:LEU:HD23	1:J:54:ILE:CG2	2.42	0.44
1:J:50:VAL:O	1:J:54:ILE:HG13	2.17	0.44
1:G:184:ALA:O	1:G:188:ILE:HG13	2.18	0.44
1:F:116:ILE:HD11	1:F:151:ILE:HD13	1.99	0.44
1:D:156:ARG:O	1:D:158:VAL:HG23	2.17	0.44
1:H:375:ALA:O	1:H:379:LYS:HG3	2.18	0.44
1:J:138:THR:HB	1:J:190:THR:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:LEU:HD12	1:E:383:LEU:C	2.43	0.44
1:A:139:ALA:H	1:A:182:LYS:NZ	2.16	0.44
1:F:83:PHE:HZ	1:F:130:VAL:HG11	1.83	0.44
1:D:92:VAL:HG22	1:D:133:VAL:HB	1.99	0.44
1:E:50:VAL:O	1:E:54:ILE:HG13	2.18	0.44
1:F:115:ARG:HD3	1:F:117:ASN:ND2	2.33	0.44
1:F:203:VAL:HG11	1:F:299:PHE:CZ	2.53	0.44
1:C:25:LEU:HD23	1:C:54:ILE:HG23	2.00	0.44
1:C:253:PHE:CD1	1:C:253:PHE:C	2.95	0.44
1:C:340:ALA:CA	1:C:382:MET:HE3	2.48	0.44
1:A:138:THR:HB	1:A:190:THR:HG21	1.99	0.44
1:I:68:GLN:NE2	1:I:75:GLN:HE22	2.16	0.44
1:I:91:LEU:HB2	1:I:132:VAL:HG22	1.99	0.44
1:I:283:ASN:HB2	1:I:339:TYR:OH	2.18	0.44
1:I:297:GLU:H	1:I:297:GLU:CD	2.25	0.44
1:E:317:ALA:O	1:E:321:ARG:HG2	2.18	0.44
1:F:197:HIS:HB2	1:F:249:ALA:HB1	2.00	0.44
1:F:244:TYR:O	1:F:248:MET:HG3	2.17	0.44
1:I:18:VAL:O	1:I:21:VAL:HG22	2.17	0.44
1:H:153:ASP:OD2	1:H:155:ALA:HB3	2.19	0.43
1:J:76:VAL:HG11	1:J:116:ILE:HG12	1.99	0.43
1:J:349:ILE:HD13	1:J:379:LYS:HG2	1.99	0.43
1:G:24:ARG:HB3	1:G:171:VAL:HG21	2.00	0.43
1:F:3:THR:HG21	1:F:208:THR:HG21	2.00	0.43
1:F:40:PHE:O	1:F:44:THR:HG23	2.18	0.43
1:C:382:MET:HE2	1:C:382:MET:HB3	1.81	0.43
1:H:15:ARG:HE	1:H:15:ARG:HB3	1.59	0.43
1:J:31:LYS:O	1:J:59:VAL:HG13	2.17	0.43
1:J:111:ALA:CB	1:J:127:LYS:HG3	2.39	0.43
1:E:341:GLU:H	1:E:341:GLU:HG3	1.51	0.43
1:F:291:ASN:O	1:F:299:PHE:HE2	2.00	0.43
1:I:281:SER:HB2	1:I:335:ILE:HG21	2.00	0.43
1:I:292:LEU:HD23	1:I:292:LEU:HA	1.86	0.43
1:G:186:LEU:O	1:G:190:THR:OG1	2.28	0.43
1:F:272:TYR:CZ	1:F:344:VAL:HA	2.53	0.43
1:C:50:VAL:HG12	1:C:54:ILE:HD11	2.00	0.43
1:C:112:ASN:CG	1:C:125:VAL:HG13	2.44	0.43
1:A:174:VAL:CG1	1:A:243:ALA:HB1	2.49	0.43
1:H:103:ALA:HA	1:H:106:ILE:HD12	1.99	0.43
1:J:52:LYS:O	1:J:56:GLU:HG3	2.19	0.43
1:J:350:GLU:O	1:J:354:LYS:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:ILE:HG22	1:E:59:VAL:HB	2.00	0.43
1:F:148:LEU:HD11	1:F:161:PRO:CB	2.49	0.43
1:C:70:ASP:OD2	1:C:152:THR:HG21	2.18	0.43
1:J:32:LYS:CG	1:J:88:CYS:HA	2.48	0.43
1:E:119:TYR:O	1:E:123:ASN:ND2	2.30	0.43
1:E:283:ASN:HB2	1:E:339:TYR:OH	2.18	0.43
1:A:164:ASP:O	1:A:167:ILE:HG12	2.18	0.43
1:I:113:GLY:N	1:I:119:TYR:OH	2.48	0.43
1:B:382:MET:HE3	1:B:382:MET:HB3	1.69	0.43
1:D:373:ASP:O	1:D:377:ILE:HG13	2.18	0.43
1:H:82:VAL:O	1:H:86:GLU:HG2	2.18	0.43
1:F:260:LEU:O	1:F:264:ILE:HD12	2.19	0.43
1:A:7:ILE:HG13	1:A:8:PRO:HD2	2.00	0.43
1:I:22:GLY:O	1:I:23:THR:C	2.59	0.43
1:I:224:GLU:HB3	1:I:225:TYR:CD2	2.54	0.43
1:H:68:GLN:OE1	1:H:69:PRO:HD2	2.19	0.43
1:E:138:THR:O	1:E:179:MET:HE2	2.19	0.43
1:E:236:ILE:O	1:E:240:GLU:HB2	2.19	0.43
1:I:40:PHE:O	1:I:44:THR:HG23	2.18	0.43
1:D:21:VAL:HG11	1:D:50:VAL:HG13	1.99	0.43
1:D:115:ARG:O	1:D:118:ASP:OD1	2.37	0.43
1:J:294:ALA:O	1:C:228:LYS:NZ	2.44	0.43
1:E:247:TYR:O	1:E:251:VAL:HG23	2.18	0.43
1:E:374:ILE:O	1:E:378:ILE:HG13	2.19	0.43
1:B:82:VAL:O	1:B:85:GLN:HG2	2.19	0.43
1:D:221:LEU:HA	1:D:221:LEU:HD23	1.77	0.43
1:H:383:LEU:HD23	1:H:383:LEU:HA	1.80	0.43
1:G:298:ARG:O	1:G:302:ILE:HG13	2.19	0.43
1:C:136:THR:HG21	1:C:246:GLN:HE22	1.83	0.43
1:A:142:GLY:H	1:A:246:GLN:HE21	1.66	0.43
1:I:25:LEU:HG	1:I:30:ALA:CB	2.42	0.43
1:H:374:ILE:O	1:H:378:ILE:HG13	2.19	0.43
1:A:289:ALA:CA	1:A:292:LEU:HD13	2.40	0.43
1:D:45:GLY:O	1:D:49:GLU:HG3	2.18	0.42
1:E:35:ILE:CD1	1:E:61:VAL:HG21	2.49	0.42
1:E:208:THR:CG2	1:E:211:THR:H	2.32	0.42
1:A:112:ASN:OD1	1:A:125:VAL:HG13	2.19	0.42
1:A:197:HIS:CD2	1:A:262:HIS:CE1	3.06	0.42
1:A:263:SER:O	1:A:267:GLN:HG2	2.19	0.42
1:A:119:TYR:O	1:A:162:VAL:HG13	2.19	0.42
1:B:138:THR:HA	1:B:182:LYS:HD2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:32:LYS:HE3	1:J:87:ASN:ND2	2.34	0.42
1:G:83:PHE:CE1	1:G:91:LEU:CD2	3.02	0.42
1:F:111:ALA:O	1:F:127:LYS:HG3	2.19	0.42
1:F:345:LYS:HB2	1:F:347:GLU:OE1	2.19	0.42
1:B:82:VAL:HA	1:B:85:GLN:HG2	2.00	0.42
1:B:297:GLU:H	1:B:297:GLU:CD	2.27	0.42
1:H:174:VAL:HG12	1:H:243:ALA:HB1	2.02	0.42
1:F:253:PHE:CD1	1:F:253:PHE:C	2.97	0.42
1:C:20:GLU:O	1:C:24:ARG:HG3	2.19	0.42
1:A:25:LEU:HD11	1:A:92:VAL:HG21	2.01	0.42
1:H:80:VAL:HG22	1:H:106:ILE:HA	2.02	0.42
1:G:260:LEU:HD23	1:G:263:SER:HB2	2.01	0.42
1:C:35:ILE:HB	1:C:63:ILE:HD13	2.01	0.42
1:A:91:LEU:HB2	1:A:132:VAL:HG22	1.99	0.42
1:I:89:ASP:O	1:I:130:VAL:HG13	2.20	0.42
1:D:78:GLU:O	1:D:81:ASP:HB2	2.19	0.42
1:D:157:LYS:HB2	1:D:157:LYS:HE3	1.75	0.42
1:F:272:TYR:OH	1:F:345:LYS:HG2	2.20	0.42
1:C:138:THR:HB	1:C:190:THR:HG21	2.02	0.42
1:A:138:THR:HA	1:A:182:LYS:HD2	2.01	0.42
1:A:313:LEU:HD22	1:A:317:ALA:HB1	2.00	0.42
1:I:100:HIS:O	1:I:104:LYS:HG3	2.20	0.42
1:I:359:ASP:OD1	1:I:360:VAL:N	2.53	0.42
1:B:310:VAL:HA	1:B:313:LEU:HD12	2.00	0.42
1:H:148:LEU:HB2	1:H:163:ILE:HG12	2.01	0.42
1:J:66:LYS:HE2	1:J:75:GLN:OE1	2.19	0.42
1:G:283:ASN:HD22	1:G:283:ASN:HA	1.64	0.42
1:C:202:TYR:CE2	1:C:298:ARG:HB3	2.54	0.42
1:I:382:MET:O	1:I:383:LEU:HD23	2.20	0.42
1:B:49:GLU:OE1	1:B:49:GLU:N	2.53	0.42
1:D:117:ASN:HA	1:D:160:MET:HE1	2.01	0.42
1:H:100:HIS:HE2	1:H:136:THR:HA	1.84	0.42
1:J:66:LYS:CE	1:J:75:GLN:OE1	2.68	0.42
1:G:182:LYS:HD2	1:G:186:LEU:HG	2.02	0.42
1:I:20:GLU:O	1:I:21:VAL:C	2.63	0.42
1:B:263:SER:OG	1:B:361:CYS:HB2	2.19	0.42
1:D:220:LYS:HG3	1:D:305:LEU:HD22	2.02	0.42
1:H:147:SER:HB3	1:H:164:ASP:O	2.20	0.42
1:J:68:GLN:HB3	1:J:75:GLN:HE21	1.85	0.42
1:J:212:ASP:O	1:J:216:ILE:HD12	2.20	0.42
1:F:116:ILE:HG12	1:F:151:ILE:HG21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ILE:HD12	1:C:119:TYR:HB2	2.00	0.42
1:C:176:PRO:HG3	1:C:240:GLU:HG2	2.01	0.42
1:D:76:VAL:HG21	1:D:151:ILE:HG12	2.02	0.42
1:D:140:GLY:N	1:D:246:GLN:HG3	2.35	0.42
1:D:226:LEU:N	1:D:227:PRO:HD2	2.35	0.42
1:D:294:ALA:HB1	1:D:366:PRO:HB2	2.01	0.42
1:H:64:PHE:CE1	1:H:79:GLY:HA2	2.55	0.42
1:H:115:ARG:HH21	1:H:117:ASN:HB2	1.83	0.42
1:F:273:LYS:HG3	1:F:273:LYS:O	2.18	0.42
1:C:258:LEU:O	1:C:364:SER:OG	2.31	0.42
1:J:119:TYR:C	1:J:162:VAL:HG22	2.45	0.41
1:J:166:LYS:HD2	1:J:166:LYS:HA	1.73	0.41
1:E:209:PRO:HB3	1:I:221:LEU:HD11	2.01	0.41
1:C:260:LEU:HA	1:C:263:SER:HB2	2.02	0.41
1:I:81:ASP:O	1:I:85:GLN:HG3	2.20	0.41
1:D:40:PHE:O	1:D:44:THR:HG23	2.20	0.41
1:J:66:LYS:HA	1:J:66:LYS:HD2	1.92	0.41
1:E:78:GLU:HA	1:E:81:ASP:OD2	2.20	0.41
1:E:103:ALA:HA	1:E:106:ILE:HD12	2.01	0.41
1:G:92:VAL:HG22	1:G:133:VAL:HB	2.02	0.41
1:F:111:ALA:HB1	1:F:127:LYS:HB3	2.02	0.41
1:F:346:GLU:HA	1:F:349:ILE:HG13	2.02	0.41
1:C:261:VAL:HA	1:C:283:ASN:OD1	2.20	0.41
1:D:15:ARG:NH1	1:D:236:ILE:HG21	2.34	0.41
1:D:22:GLY:O	1:D:23:THR:C	2.63	0.41
1:H:20:GLU:O	1:H:21:VAL:C	2.62	0.41
1:H:58:GLY:O	1:H:59:VAL:CB	2.68	0.41
1:G:4:ASN:ND2	1:F:24:ARG:HH21	2.18	0.41
1:G:63:ILE:C	1:G:65:PRO:HD3	2.45	0.41
1:C:210:VAL:H	1:C:210:VAL:HG23	1.63	0.41
1:I:68:GLN:O	1:I:98:SER:HB2	2.20	0.41
1:B:63:ILE:HG22	1:B:65:PRO:HD3	2.03	0.41
1:D:346:GLU:H	1:D:346:GLU:CD	2.27	0.41
1:H:247:TYR:O	1:H:251:VAL:HG23	2.20	0.41
1:H:346:GLU:OE2	1:H:346:GLU:N	2.31	0.41
1:G:142:GLY:H	1:G:246:GLN:HE21	1.68	0.41
1:F:117:ASN:OD1	1:F:117:ASN:C	2.63	0.41
1:F:263:SER:OG	1:F:361:CYS:HB2	2.21	0.41
1:F:341:GLU:H	1:F:341:GLU:HG3	1.75	0.41
1:A:31:LYS:H	1:A:89:ASP:CG	2.27	0.41
1:A:32:LYS:HA	1:A:60:ASP:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:156:ARG:O	1:H:158:VAL:HG23	2.20	0.41
1:J:20:GLU:O	1:J:21:VAL:C	2.64	0.41
1:G:20:GLU:O	1:G:21:VAL:C	2.63	0.41
1:C:375:ALA:HA	1:C:378:ILE:HD12	2.03	0.41
1:I:50:VAL:HG12	1:I:54:ILE:HD11	2.03	0.41
1:I:373:ASP:O	1:I:377:ILE:HG13	2.21	0.41
1:D:150:VAL:HG23	1:D:150:VAL:O	2.20	0.41
1:J:199:ILE:O	1:J:203:VAL:HG22	2.21	0.41
1:E:71:PRO:CG	1:E:98:SER:HA	2.50	0.41
1:G:338:GLY:HA3	1:G:382:MET:O	2.20	0.41
1:F:281:SER:HB2	1:F:335:ILE:HG21	2.02	0.41
1:C:108:LEU:O	1:C:108:LEU:HD12	2.21	0.41
1:A:382:MET:HE3	1:A:382:MET:HB3	1.77	0.41
1:D:382:MET:HB3	1:D:382:MET:HE3	1.58	0.41
1:H:205:LYS:HE2	1:H:363:GLN:O	2.20	0.41
1:J:35:ILE:HD11	1:J:54:ILE:HD12	2.02	0.41
1:J:76:VAL:O	1:J:80:VAL:HG23	2.20	0.41
1:J:261:VAL:HG23	1:J:287:VAL:HG11	2.01	0.41
1:G:284:MET:HE3	1:G:284:MET:HB2	1.92	0.41
1:G:313:LEU:HD23	1:G:313:LEU:HA	1.90	0.41
1:C:136:THR:HG22	1:C:138:THR:H	1.85	0.41
1:I:146:THR:HG21	1:I:253:PHE:CZ	2.55	0.41
1:B:144:GLU:HG2	1:B:145:THR:HG23	2.03	0.41
1:H:317:ALA:O	1:H:321:ARG:HG2	2.21	0.41
1:G:21:VAL:HG13	1:G:22:GLY:N	2.36	0.41
1:G:139:ALA:H	1:G:182:LYS:NZ	2.19	0.41
1:F:23:THR:OG1	1:F:24:ARG:N	2.53	0.41
1:F:382:MET:HE3	1:F:382:MET:HB3	1.79	0.41
1:C:226:LEU:N	1:C:227:PRO:HD2	2.36	0.41
1:A:340:ALA:HB2	1:A:382:MET:HE3	2.02	0.41
1:I:51:ALA:HA	1:I:54:ILE:HD12	2.03	0.41
1:B:68:GLN:O	1:B:98:SER:HB3	2.20	0.41
1:B:84:LYS:HG2	1:B:84:LYS:H	1.62	0.41
1:B:176:PRO:HG3	1:B:240:GLU:HG2	2.02	0.41
1:B:240:GLU:OE2	1:D:1:MET:HG3	2.20	0.41
1:D:20:GLU:O	1:D:21:VAL:C	2.64	0.41
1:E:276:HIS:CE1	1:E:280:ASN:HD21	2.39	0.41
1:G:149:ALA:N	1:G:163:ILE:HD13	2.34	0.41
1:G:263:SER:OG	1:G:362:THR:HG23	2.21	0.41
1:C:5:PHE:HB3	1:A:11:SER:HB2	2.03	0.41
1:C:302:ILE:O	1:C:306:LEU:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:41:LEU:HD22	1:J:46:LEU:HD23	2.03	0.41
1:J:103:ALA:HA	1:J:106:ILE:CD1	2.51	0.41
1:F:69:PRO:HB2	1:F:273:LYS:NZ	2.36	0.41
1:C:82:VAL:O	1:C:86:GLU:HG2	2.21	0.41
1:A:32:LYS:HG2	1:A:88:CYS:SG	2.61	0.41
1:B:14:GLY:C	1:B:176:PRO:HD2	2.46	0.40
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.86	0.40
1:D:33:ALA:O	1:D:61:VAL:HA	2.21	0.40
1:D:50:VAL:HG21	1:D:94:ILE:HD13	2.02	0.40
1:J:7:ILE:HD12	1:J:251:VAL:CG1	2.48	0.40
1:J:197:HIS:CD2	1:J:262:HIS:CE1	3.09	0.40
1:G:228:LYS:NZ	1:I:294:ALA:O	2.54	0.40
1:A:340:ALA:HB3	1:A:383:LEU:HD21	2.03	0.40
1:D:227:PRO:HB2	1:E:293:ILE:O	2.21	0.40
1:E:199:ILE:O	1:E:203:VAL:HG22	2.20	0.40
1:G:336:PRO:CB	1:G:342:MET:HE2	2.43	0.40
1:G:373:ASP:O	1:G:377:ILE:HG13	2.21	0.40
1:A:345:LYS:HD2	1:A:348:ASP:OD2	2.22	0.40
1:B:168:THR:HA	1:B:169:PRO:HD3	1.98	0.40
1:H:111:ALA:HB1	1:H:127:LYS:HB3	2.04	0.40
1:J:31:LYS:CD	1:J:32:LYS:HG2	2.51	0.40
1:J:182:LYS:HE2	1:J:182:LYS:HB3	1.75	0.40
1:D:70:ASP:O	1:D:71:PRO:C	2.63	0.40
1:J:66:LYS:O	1:J:67:ALA:C	2.64	0.40
1:A:120:GLN:HG3	1:A:160:MET:HB3	2.04	0.40
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.94	0.40
1:H:32:LYS:HE2	1:H:88:CYS:SG	2.62	0.40
1:H:120:GLN:HA	1:H:162:VAL:HG22	2.03	0.40
1:E:104:LYS:HB3	1:E:167:ILE:HB	2.04	0.40
1:E:159:LYS:HD3	1:E:266:HIS:HA	2.04	0.40
1:A:21:VAL:HG13	1:A:22:GLY:N	2.36	0.40
1:A:321:ARG:HG2	1:A:321:ARG:H	1.69	0.40
1:I:34:LEU:HD12	1:I:34:LEU:HA	1.83	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:G:346:GLU:OE2	1:F:354:LYS:NZ[1_565]	2.16	0.04

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%)	368 (96%)	13 (3%)	1 (0%)	37	70
1	B	383/390 (98%)	368 (96%)	14 (4%)	1 (0%)	37	70
1	C	382/390 (98%)	365 (96%)	16 (4%)	1 (0%)	37	70
1	D	382/390 (98%)	363 (95%)	18 (5%)	1 (0%)	37	70
1	E	382/390 (98%)	363 (95%)	18 (5%)	1 (0%)	37	70
1	F	382/390 (98%)	366 (96%)	13 (3%)	3 (1%)	16	51
1	G	319/390 (82%)	300 (94%)	15 (5%)	4 (1%)	10	39
1	H	382/390 (98%)	367 (96%)	12 (3%)	3 (1%)	16	51
1	I	382/390 (98%)	367 (96%)	13 (3%)	2 (0%)	25	61
1	J	382/390 (98%)	354 (93%)	22 (6%)	6 (2%)	8	34
All	All	3758/3900 (96%)	3581 (95%)	154 (4%)	23 (1%)	22	57

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	59	VAL
1	J	97	GLY
1	J	112	ASN
1	D	125	VAL
1	J	66	LYS
1	G	63	ILE
1	G	65	PRO
1	H	111	ALA
1	F	154	SER
1	J	110	ALA
1	E	125	VAL
1	C	125	VAL
1	I	125	VAL
1	B	125	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	382	MET
1	G	69	PRO
1	F	125	VAL
1	A	125	VAL
1	I	115	ARG
1	H	125	VAL
1	G	64	PHE
1	J	125	VAL
1	F	35	ILE

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%)	300 (100%)	0	100	100
1	B	301/306 (98%)	301 (100%)	0	100	100
1	C	300/306 (98%)	300 (100%)	0	100	100
1	D	300/306 (98%)	300 (100%)	0	100	100
1	E	300/306 (98%)	300 (100%)	0	100	100
1	F	300/306 (98%)	300 (100%)	0	100	100
1	G	255/306 (83%)	255 (100%)	0	100	100
1	H	300/306 (98%)	300 (100%)	0	100	100
1	I	300/306 (98%)	300 (100%)	0	100	100
1	J	300/306 (98%)	299 (100%)	1 (0%)	91	96
All	All	2956/3060 (97%)	2955 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	167	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	246	GLN
1	B	283	ASN
1	B	363	GLN
1	D	4	ASN
1	D	85	GLN
1	D	112	ASN
1	D	117	ASN
1	D	286	HIS
1	H	117	ASN
1	H	120	GLN
1	H	232	ASN
1	J	87	ASN
1	J	223	ASN
1	J	266	HIS
1	J	283	ASN
1	J	355	ASN
1	E	68	GLN
1	E	120	GLN
1	E	223	ASN
1	E	246	GLN
1	E	266	HIS
1	E	283	ASN
1	E	291	ASN
1	E	365	ASN
1	G	223	ASN
1	G	286	HIS
1	F	68	GLN
1	F	77	HIS
1	F	87	ASN
1	F	217	GLN
1	C	75	GLN
1	C	283	ASN
1	C	286	HIS
1	C	376	GLN
1	A	87	ASN
1	A	120	GLN
1	A	123	ASN
1	A	246	GLN
1	A	283	ASN
1	I	68	GLN
1	I	77	HIS
1	I	232	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	384/390 (98%)	-0.60	1 (0%) 90 81	31, 50, 67, 90	0
1	B	384/390 (98%)	-0.62	1 (0%) 90 81	31, 47, 69, 95	1 (0%)
1	C	384/390 (98%)	-0.49	0 100 100	32, 54, 77, 102	0
1	D	384/390 (98%)	-0.32	3 (0%) 82 66	34, 53, 100, 115	0
1	E	384/390 (98%)	-0.39	2 (0%) 87 75	31, 53, 94, 128	0
1	F	384/390 (98%)	-0.20	9 (2%) 61 39	34, 56, 110, 122	0
1	G	329/390 (84%)	-0.38	6 (1%) 67 45	30, 50, 109, 130	0
1	H	384/390 (98%)	-0.25	4 (1%) 79 60	35, 59, 114, 131	0
1	I	384/390 (98%)	-0.56	0 100 100	30, 47, 82, 108	0
1	J	384/390 (98%)	-0.04	17 (4%) 39 23	39, 66, 136, 153	0
All	All	3785/3900 (97%)	-0.39	43 (1%) 77 58	30, 52, 108, 153	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	121	GLY	5.1
1	F	108	LEU	4.8
1	J	161	PRO	4.5
1	G	83	PHE	4.1
1	F	88	CYS	3.6
1	E	116	ILE	3.6
1	B	1	MET	3.4
1	J	150	VAL	3.4
1	G	105	ALA	3.3
1	G	61	VAL	3.3
1	G	63	ILE	3.3
1	J	162	VAL	3.2
1	J	160	MET	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	59	VAL	2.9
1	J	116	ILE	2.9
1	J	151	ILE	2.8
1	J	163	ILE	2.6
1	J	34	LEU	2.6
1	F	2	THR	2.6
1	D	116	ILE	2.6
1	H	108	LEU	2.6
1	F	34	LEU	2.6
1	F	158	VAL	2.5
1	H	152	THR	2.5
1	F	109	VAL	2.5
1	F	70	ASP	2.4
1	D	109	VAL	2.4
1	J	70	ASP	2.4
1	E	73	ASP	2.4
1	G	30	ALA	2.4
1	J	67	ALA	2.4
1	A	1	MET	2.4
1	H	122	VAL	2.3
1	F	107	GLY	2.3
1	J	88	CYS	2.2
1	J	108	LEU	2.2
1	F	121	GLY	2.1
1	D	161	PRO	2.1
1	H	128	PRO	2.1
1	J	90	SER	2.0
1	J	61	VAL	2.0
1	J	107	GLY	2.0
1	J	69	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	I	402	1/1	0.79	0.17	96,96,96,96	0
3	CL	E	402	1/1	0.96	0.05	64,64,64,64	0
2	MN	E	401	1/1	0.97	0.06	38,38,38,38	0
2	MN	D	401	1/1	0.98	0.04	48,48,48,48	0
2	MN	H	401	1/1	0.98	0.05	43,43,43,43	0
2	MN	J	401	1/1	0.98	0.07	53,53,53,53	0
2	MN	C	401	1/1	0.99	0.03	46,46,46,46	0
2	MN	A	401	1/1	0.99	0.04	47,47,47,47	0
2	MN	I	401	1/1	0.99	0.06	44,44,44,44	0
2	MN	B	401	1/1	0.99	0.04	41,41,41,41	0
2	MN	G	401	1/1	0.99	0.05	42,42,42,42	0
2	MN	F	401	1/1	1.00	0.03	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.