



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 08:37 PM EDT

PDB ID : 3TUJ
Title : Inward facing conformations of the MetNI methionine ABC transporter: DM crystal form
Authors : Johnson, E.; Nguyen, P.; Rees, D.C.
Deposited on : 2011-09-16
Resolution : 4.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

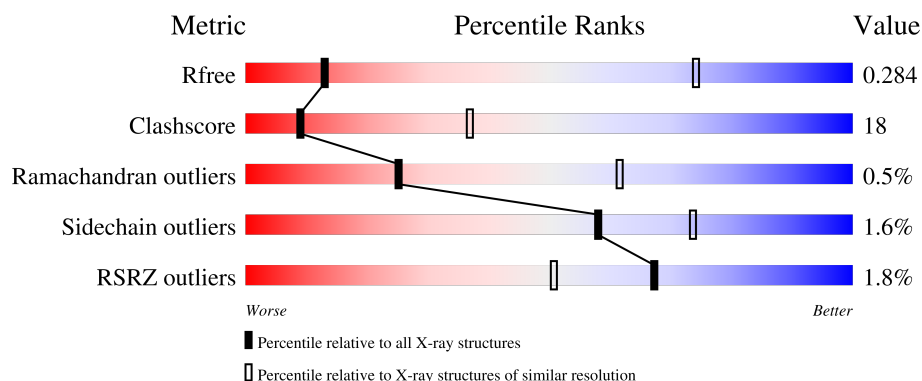
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1028 (4.22-3.78)
Clashscore	180529	1055 (4.20-3.80)
Ramachandran outliers	177936	1004 (4.20-3.80)
Sidechain outliers	177891	1027 (4.22-3.78)
RSRZ outliers	164620	1029 (4.22-3.78)

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	217	<div> <div>0.2%</div> <div>64%</div> <div>35%</div> </div>
1	B	217	<div> <div>0.2%</div> <div>58%</div> <div>41%</div> <div>0.1%</div> </div>
2	C	366	<div> <div>0.2%</div> <div>66%</div> <div>26%</div> <div>6%</div> </div>
2	D	366	<div> <div>3%</div> <div>62%</div> <div>31%</div> <div>6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8559 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 D-methionine transport system permease protein metI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	Se	0	0	0
			1621	1076	263	272	10			
1	B	215	Total	C	N	O	Se	0	0	0
			1616	1073	262	271	10			

- Molecule 2 is a protein called Methionine import ATP-binding protein MetN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	344	Total	C	N	O	S	Se	0	0
			2661	1670	471	508	5	7		
2	D	344	Total	C	N	O	S	Se	0	0
			2661	1670	471	508	5	7		

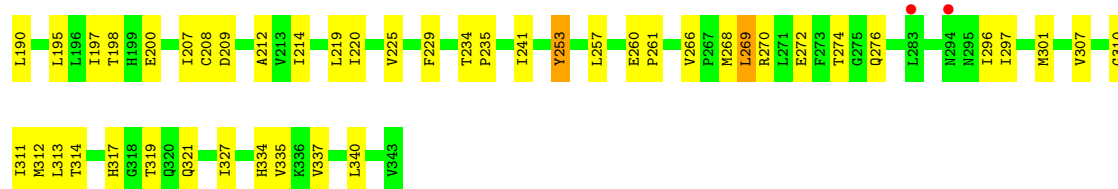
There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MSE	-	expression tag	UNP P30750
C	-21	GLY	-	expression tag	UNP P30750
C	-20	HIS	-	expression tag	UNP P30750
C	-19	HIS	-	expression tag	UNP P30750
C	-18	HIS	-	expression tag	UNP P30750
C	-17	HIS	-	expression tag	UNP P30750
C	-16	HIS	-	expression tag	UNP P30750
C	-15	HIS	-	expression tag	UNP P30750
C	-14	HIS	-	expression tag	UNP P30750
C	-13	HIS	-	expression tag	UNP P30750
C	-12	HIS	-	expression tag	UNP P30750
C	-11	HIS	-	expression tag	UNP P30750
C	-10	SER	-	expression tag	UNP P30750
C	-9	SER	-	expression tag	UNP P30750
C	-8	GLY	-	expression tag	UNP P30750
C	-7	HIS	-	expression tag	UNP P30750

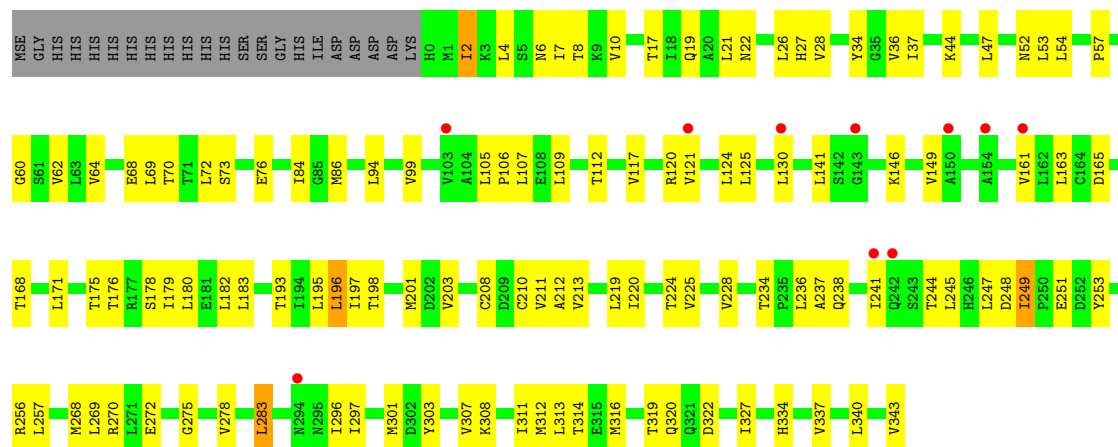
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ILE	-	expression tag	UNP P30750
C	-5	ASP	-	expression tag	UNP P30750
C	-4	ASP	-	expression tag	UNP P30750
C	-3	ASP	-	expression tag	UNP P30750
C	-2	ASP	-	expression tag	UNP P30750
C	-1	LYS	-	expression tag	UNP P30750
C	0	HIS	-	expression tag	UNP P30750
C	166	GLN	GLU	engineered mutation	UNP P30750
D	-22	MSE	-	expression tag	UNP P30750
D	-21	GLY	-	expression tag	UNP P30750
D	-20	HIS	-	expression tag	UNP P30750
D	-19	HIS	-	expression tag	UNP P30750
D	-18	HIS	-	expression tag	UNP P30750
D	-17	HIS	-	expression tag	UNP P30750
D	-16	HIS	-	expression tag	UNP P30750
D	-15	HIS	-	expression tag	UNP P30750
D	-14	HIS	-	expression tag	UNP P30750
D	-13	HIS	-	expression tag	UNP P30750
D	-12	HIS	-	expression tag	UNP P30750
D	-11	HIS	-	expression tag	UNP P30750
D	-10	SER	-	expression tag	UNP P30750
D	-9	SER	-	expression tag	UNP P30750
D	-8	GLY	-	expression tag	UNP P30750
D	-7	HIS	-	expression tag	UNP P30750
D	-6	ILE	-	expression tag	UNP P30750
D	-5	ASP	-	expression tag	UNP P30750
D	-4	ASP	-	expression tag	UNP P30750
D	-3	ASP	-	expression tag	UNP P30750
D	-2	ASP	-	expression tag	UNP P30750
D	-1	LYS	-	expression tag	UNP P30750
D	0	HIS	-	expression tag	UNP P30750
D	166	GLN	GLU	engineered mutation	UNP P30750



● Molecule 2: Methionine import ATP-binding protein MetN



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	155.75Å 164.13Å 212.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.85 – 4.00 19.85 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.85-4.00) 97.1 (19.85-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 3.82Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.259 , 0.295 0.248 , 0.284	Depositor DCC
R_{free} test set	1665 reflections (7.35%)	wwPDB-VP
Wilson B-factor (Å ²)	153.5	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 84.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8559	wwPDB-VP
Average B, all atoms (Å ²)	190.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	0/1645	0.71	0/2233
1	B	0.63	0/1640	0.67	2/2226 (0.1%)
2	C	0.58	1/2694 (0.0%)	0.66	1/3641 (0.0%)
2	D	0.53	0/2694	0.60	0/3641
All	All	0.61	1/8673 (0.0%)	0.65	3/11741 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	MSE	CG-SE	-5.06	1.78	1.95

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	131	GLY	N-CA-C	-6.94	95.76	113.10
1	B	163	MSE	CG-SE-CE	6.16	112.45	98.90
1	B	107	MSE	CB-CG-SE	-6.12	94.34	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1621	0	1735	83	0
1	B	1616	0	1733	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2661	0	2714	75	0
2	D	2661	0	2714	102	0
All	All	8559	0	8896	315	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (315) 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:A:163:MSE:SE	1:B:163:MSE:HG3	1.95	1.16
1:B:147:VAL:HG23	1:B:211:VAL:HG22	1.40	1.03
1:A:69:ILE:HG21	1:B:163:MSE:CE	1.90	1.00
1:A:143:LEU:HD22	1:A:214:VAL:HG21	1.47	0.94
1:B:104:ILE:HG22	1:B:153:THR:HG21	1.52	0.92
2:D:107:LEU:HD23	2:D:117:VAL:HG23	1.52	0.91
1:A:69:ILE:HG21	1:B:163:MSE:HE2	1.51	0.91
2:D:37:ILE:HD13	2:D:201:MSE:HE2	1.54	0.89
1:B:104:ILE:CG2	1:B:153:THR:HG21	2.04	0.86
1:A:128:ALA:HB2	2:C:109:LEU:HD21	1.57	0.85
2:D:198:THR:HG21	2:D:203:VAL:HG11	1.59	0.85
2:D:64:VAL:HG11	2:D:84:ILE:HD11	1.59	0.82
1:B:154:LEU:HD23	1:B:203:ILE:HG23	1.63	0.81
1:A:19:MSE:HE2	1:A:96:LEU:HD11	1.64	0.79
2:D:249:ILE:HG22	2:D:313:LEU:HD11	1.64	0.79
1:A:187:THR:O	1:A:188:VAL:HG12	1.82	0.78
1:A:19:MSE:CE	1:A:96:LEU:HD11	2.13	0.78
2:D:256:ARG:HD2	2:D:343:VAL:HG23	1.65	0.77
1:A:163:MSE:HB3	1:B:163:MSE:HE3	1.66	0.76
1:A:162:ALA:HB1	1:B:70:ILE:HD13	1.68	0.76
2:C:253:TYR:CD2	2:C:268:MSE:HE1	2.21	0.76
2:D:241:ILE:O	2:D:244:THR:HG22	1.86	0.76
1:A:133:ILE:HG22	1:A:138:LEU:HD13	1.66	0.75
1:A:92:ALA:HB2	1:A:169:ALA:HB1	1.69	0.74
1:B:75:MSE:HE1	1:B:98:VAL:HG11	1.70	0.73
1:B:19:MSE:HE2	1:B:96:LEU:HD11	1.68	0.73
2:D:130:LEU:HD13	2:D:149:VAL:HG12	1.71	0.73
2:D:168:THR:HG21	2:D:180:LEU:HD12	1.68	0.73
1:B:17:LEU:HD21	1:B:199:LEU:HD11	1.71	0.72
1:A:20:THR:HG21	1:A:158:VAL:HG22	1.70	0.72
2:D:10:VAL:HG11	2:D:17:THR:HG23	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:LEU:HD13	2:D:7:ILE:HD13	1.72	0.72
2:C:103:VAL:HG21	2:C:125:LEU:HD11	1.72	0.71
2:C:131:GLY:O	2:C:133:LYS:N	2.25	0.70
1:A:69:ILE:CG2	1:B:163:MSE:CE	2.68	0.69
2:C:229:PHE:CD2	2:C:241:ILE:HD11	2.27	0.69
2:D:180:LEU:HD21	2:D:203:VAL:HG13	1.74	0.69
2:C:297:ILE:HG22	2:C:313:LEU:O	1.92	0.69
1:B:20:THR:HG21	1:B:158:VAL:HG22	1.73	0.69
2:D:171:LEU:HD23	2:D:175:THR:HG22	1.74	0.68
2:D:28:VAL:HG22	2:D:34:TYR:CD2	2.28	0.68
1:B:123:SER:HA	1:B:126:MSE:HE2	1.74	0.68
1:A:137:VAL:HG13	2:C:94:LEU:HD21	1.75	0.67
2:C:10:VAL:HG12	2:C:19:GLN:HA	1.77	0.66
2:D:249:ILE:HG22	2:D:313:LEU:CD1	2.24	0.66
2:D:275:GLY:C	2:D:307:VAL:HG21	2.16	0.66
1:B:41:THR:HG21	1:B:52:LEU:HD11	1.77	0.64
1:B:129:THR:HG22	1:B:132:GLN:HG3	1.79	0.64
1:B:147:VAL:CG2	1:B:211:VAL:HG22	2.21	0.64
2:D:168:THR:HG21	2:D:180:LEU:CD1	2.27	0.64
1:A:117:THR:O	1:A:120:ILE:HG22	1.97	0.64
2:D:248:ASP:O	2:D:249:ILE:HG13	1.97	0.64
1:B:5:MSE:HE1	1:B:179:TYR:CZ	2.32	0.64
2:C:12:HIS:HB3	2:C:17:THR:HG22	1.80	0.64
2:D:253:TYR:CE2	2:D:297:ILE:HD13	2.33	0.64
1:A:21:PHE:CE2	1:A:154:LEU:HD11	2.33	0.63
1:A:97:THR:O	1:A:98:VAL:HB	1.99	0.63
2:C:168:THR:HG23	2:C:176:THR:CG2	2.28	0.63
2:C:171:LEU:HB3	2:C:175:THR:HG23	1.81	0.62
2:C:301:MSE:HE2	2:C:312:MSE:HE3	1.81	0.62
1:B:5:MSE:HE1	1:B:179:TYR:OH	1.99	0.62
2:C:24:VAL:HG13	2:C:219:LEU:HB2	1.79	0.62
2:D:107:LEU:HG	2:D:112:THR:HG21	1.81	0.62
1:A:32:LEU:HD12	1:A:108:VAL:HG11	1.81	0.61
2:D:10:VAL:CG1	2:D:17:THR:HG23	2.31	0.61
1:A:85:THR:HG23	1:A:91:ALA:HB2	1.83	0.61
2:C:301:MSE:CE	2:C:312:MSE:HE3	2.31	0.61
2:D:272:GLU:HG2	2:D:311:ILE:HG22	1.81	0.61
2:D:36:VAL:HB	2:D:197:ILE:HG22	1.84	0.60
2:C:180:LEU:HD22	2:C:207:ILE:HD13	1.83	0.60
2:C:48:ILE:HD12	2:C:197:ILE:HG12	1.84	0.60
2:C:297:ILE:HD11	2:D:303:TYR:CD1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:245:LEU:HD12	2:D:311:ILE:HG23	1.85	0.59
2:D:296:ILE:HA	2:D:314:THR:HG22	1.83	0.59
2:D:249:ILE:HD12	2:D:249:ILE:O	2.03	0.58
1:A:25:PHE:O	1:A:29:VAL:HG23	2.04	0.58
1:A:155:ILE:HG22	1:A:203:ILE:CD1	2.33	0.58
1:A:69:ILE:CG2	1:B:163:MSE:HE3	2.33	0.58
2:C:28:VAL:HG22	2:C:34:TYR:CD2	2.39	0.58
1:A:82:ILE:HG23	1:A:83:VAL:HG23	1.84	0.58
1:A:69:ILE:HG21	1:B:163:MSE:HE3	1.83	0.58
1:A:101:ALA:HB3	1:A:102:PRO:CD	2.34	0.58
2:C:163:LEU:HD23	2:C:195:LEU:HB2	1.86	0.57
1:B:104:ILE:HG23	1:B:153:THR:HG21	1.85	0.57
2:C:64:VAL:HG11	2:C:84:ILE:HD11	1.87	0.57
2:D:301:MSE:HE2	2:D:312:MSE:CE	2.35	0.57
1:A:19:MSE:HE3	1:A:92:ALA:HB1	1.86	0.56
1:A:69:ILE:CG2	1:B:163:MSE:HE2	2.31	0.56
1:A:172:LEU:HG	1:A:192:VAL:HG23	1.86	0.56
1:B:78:PHE:CE2	1:B:82:ILE:HD11	2.40	0.56
1:B:23:SER:HB2	1:B:157:LEU:HD13	1.86	0.56
1:B:19:MSE:CE	1:B:96:LEU:HD11	2.36	0.56
1:A:20:THR:HG21	1:A:158:VAL:CG2	2.35	0.56
2:C:319:THR:HG22	2:C:321:GLN:H	1.70	0.56
1:B:207:GLY:O	1:B:211:VAL:HG23	2.05	0.56
2:D:168:THR:HB	2:D:176:THR:HG23	1.87	0.56
1:B:182:ILE:HD12	1:B:183:GLY:N	2.21	0.56
1:B:100:ALA:HB2	1:B:157:LEU:HD21	1.88	0.55
2:C:2:ILE:CG2	2:C:161:VAL:HG21	2.37	0.55
2:C:212:ALA:HB1	2:C:219:LEU:HD11	1.88	0.55
2:D:120:ARG:O	2:D:124:LEU:HD13	2.07	0.55
1:B:120:ILE:HD11	1:B:133:ILE:HD12	1.89	0.55
2:C:297:ILE:HD13	2:D:278:VAL:HG21	1.89	0.55
1:A:181:TYR:CE1	1:B:167:VAL:HG13	2.41	0.55
1:B:133:ILE:HA	1:B:137:VAL:HG22	1.89	0.54
1:A:181:TYR:CD1	1:B:167:VAL:HG13	2.42	0.54
1:A:80:ARG:O	1:A:84:GLY:HA2	2.06	0.54
2:C:229:PHE:CG	2:C:241:ILE:HD11	2.42	0.54
2:D:224:THR:O	2:D:228:VAL:HG23	2.07	0.54
1:B:128:ALA:HB2	2:D:109:LEU:HD11	1.90	0.54
1:A:123:SER:HA	1:A:126:MSE:HE2	1.90	0.53
1:B:22:VAL:HG11	1:B:93:ILE:HG21	1.90	0.53
1:B:78:PHE:CZ	1:B:82:ILE:HD11	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:GLU:HB3	2:C:261:PRO:CD	2.38	0.53
2:D:54:LEU:HD11	2:D:86:MSE:SE	2.59	0.53
1:A:21:PHE:CD2	1:A:154:LEU:HD11	2.43	0.53
2:D:311:ILE:HD12	2:D:311:ILE:C	2.29	0.53
1:A:94:VAL:HB	1:A:95:PRO:HD3	1.91	0.52
1:B:172:LEU:HB3	1:B:192:VAL:HG13	1.92	0.52
2:C:296:ILE:HA	2:C:314:THR:HG22	1.92	0.52
1:B:129:THR:OG1	1:B:130:PRO:HD2	2.08	0.52
2:D:179:ILE:O	2:D:183:LEU:HD23	2.09	0.52
1:A:214:VAL:HG22	1:A:214:VAL:O	2.10	0.52
2:C:260:GLU:HB3	2:C:261:PRO:HD2	1.92	0.52
2:D:105:LEU:N	2:D:106:PRO:HD2	2.24	0.52
2:D:26:LEU:HD23	2:D:27:HIS:N	2.25	0.51
1:B:15:GLU:HA	1:B:89:LEU:HD21	1.91	0.51
2:C:104:ALA:HB2	2:C:121:VAL:HG21	1.92	0.51
2:C:107:LEU:HD23	2:C:112:THR:HG21	1.93	0.51
2:D:253:TYR:HB3	2:D:268:MSE:HE1	1.92	0.51
1:B:93:ILE:HA	1:B:96:LEU:HD12	1.93	0.51
2:C:220:ILE:HG21	2:C:234:THR:HG21	1.92	0.51
1:A:19:MSE:HE3	1:A:96:LEU:HD11	1.89	0.50
1:A:83:VAL:HG21	1:A:91:ALA:HA	1.93	0.50
2:C:276:GLN:OE1	2:C:335:VAL:HG22	2.11	0.50
1:A:212:ARG:O	1:A:215:THR:HG22	2.11	0.50
1:B:101:ALA:HB3	1:B:102:PRO:CD	2.41	0.50
2:C:209:ASP:O	2:C:225:VAL:HG23	2.12	0.50
1:B:41:THR:CB	1:B:52:LEU:HD11	2.42	0.50
2:D:247:LEU:HD22	2:D:270:ARG:HD2	1.92	0.50
2:D:269:LEU:HD22	2:D:316:MSE:HE3	1.94	0.50
1:B:119:LEU:HD11	2:D:94:LEU:HD23	1.93	0.50
2:D:210:CYS:SG	2:D:224:THR:HG22	2.52	0.50
2:D:21:LEU:HD21	2:D:47:LEU:HB2	1.94	0.49
2:C:257:LEU:HD11	2:C:340:LEU:O	2.12	0.49
2:D:8:THR:HG23	2:D:22:ASN:HA	1.95	0.49
2:D:37:ILE:HG21	2:D:201:MSE:HE1	1.93	0.49
1:A:13:VAL:HG12	1:A:172:LEU:HD21	1.94	0.49
2:D:84:ILE:HG23	2:D:163:LEU:HD13	1.93	0.49
1:A:26:PHE:O	1:A:30:ILE:HG22	2.12	0.49
1:A:80:ARG:O	1:A:84:GLY:CA	2.61	0.49
1:B:1:MSE:N	1:B:187:THR:HG21	2.27	0.49
1:B:41:THR:CG2	1:B:52:LEU:HD11	2.42	0.49
2:C:87:ILE:HD11	2:C:164:CYS:SG	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:LEU:C	2:D:196:LEU:HD22	2.33	0.49
2:C:168:THR:HG23	2:C:176:THR:HG22	1.93	0.49
1:A:155:ILE:HG22	1:A:203:ILE:HG13	1.95	0.49
2:D:245:LEU:HD22	2:D:245:LEU:N	2.28	0.49
2:D:37:ILE:HD13	2:D:201:MSE:CE	2.34	0.48
2:D:249:ILE:O	2:D:249:ILE:CG1	2.61	0.48
1:B:32:LEU:HD12	1:B:108:VAL:HG11	1.95	0.48
2:C:172:ASP:O	2:C:176:THR:HG23	2.13	0.48
2:D:2:ILE:HD12	2:D:161:VAL:HG11	1.95	0.48
2:D:62:VAL:O	2:D:68:GLU:HA	2.13	0.48
1:B:107:MSE:HE1	1:B:149:ALA:HA	1.96	0.48
2:D:171:LEU:HD23	2:D:175:THR:CG2	2.42	0.48
1:B:1:MSE:HG3	1:B:2:SER:H	1.77	0.48
2:C:26:LEU:CD2	2:C:28:VAL:HG23	2.43	0.48
2:C:105:LEU:N	2:C:106:PRO:CD	2.77	0.48
1:B:9:LEU:HD12	1:B:175:ILE:HD13	1.96	0.48
1:A:66:ILE:HD13	1:B:193:LEU:HD11	1.95	0.48
2:C:86:MSE:HE2	2:C:163:LEU:HD13	1.96	0.48
1:A:154:LEU:CD2	1:A:203:ILE:HD12	2.44	0.47
1:B:185:ASN:ND2	1:B:188:VAL:HG23	2.28	0.47
2:C:234:THR:CG2	2:C:235:PRO:HD2	2.44	0.47
2:D:10:VAL:HG22	2:D:19:GLN:HG2	1.96	0.47
2:D:301:MSE:HE2	2:D:312:MSE:HE1	1.96	0.47
1:A:143:LEU:CD2	1:A:214:VAL:HG11	2.44	0.47
1:B:143:LEU:N	1:B:144:PRO:HD2	2.29	0.47
2:C:297:ILE:HG22	2:C:313:LEU:C	2.35	0.47
2:C:269:LEU:HD13	2:C:269:LEU:N	2.29	0.47
1:A:32:LEU:HB3	1:A:33:PRO:HD3	1.97	0.47
1:A:189:MSE:HE2	1:B:74:TRP:N	2.29	0.47
1:B:78:PHE:O	1:B:81:VAL:HG22	2.15	0.47
2:D:301:MSE:HE2	2:D:312:MSE:HE3	1.97	0.47
1:A:76:ILE:HB	1:A:77:PRO:HD3	1.96	0.47
1:B:32:LEU:N	1:B:33:PRO:CD	2.78	0.47
1:B:46:ILE:CD1	1:B:133:ILE:HD11	2.45	0.47
2:C:1:MSE:HE2	2:C:160:LYS:HB2	1.96	0.47
1:A:143:LEU:N	1:A:144:PRO:HD2	2.30	0.47
1:B:115:ILE:C	1:B:115:ILE:HD12	2.35	0.47
2:D:234:THR:HB	2:D:237:ALA:HB3	1.97	0.47
2:D:212:ALA:HB1	2:D:219:LEU:HD11	1.97	0.46
2:D:178:SER:O	2:D:182:LEU:HD13	2.16	0.46
1:A:139:LEU:N	1:A:140:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:211:VAL:CG1	2:D:228:VAL:HG21	2.46	0.46
1:B:20:THR:HG21	1:B:158:VAL:CG2	2.43	0.46
2:D:94:LEU:CD1	2:D:105:LEU:HD22	2.46	0.46
1:A:163:MSE:HB3	1:B:163:MSE:CE	2.40	0.46
1:B:46:ILE:HD11	1:B:120:ILE:HD11	1.97	0.46
1:B:118:GLY:H	1:B:120:ILE:HG22	1.80	0.46
1:B:134:VAL:O	1:B:139:LEU:HD23	2.16	0.46
2:C:270:ARG:HB3	2:C:313:LEU:HD13	1.98	0.46
2:C:198:THR:HG22	2:C:200:GLU:H	1.80	0.46
2:C:297:ILE:CD1	2:D:278:VAL:HG21	2.45	0.46
2:C:4:LEU:HD21	2:C:51:VAL:HG22	1.98	0.46
2:D:73:SER:HB3	2:D:76:GLU:HB2	1.97	0.46
1:B:25:PHE:O	1:B:29:VAL:HG23	2.16	0.45
2:C:33:ILE:HB	2:C:208:CYS:HA	1.97	0.45
2:C:62:VAL:HG12	2:C:69:LEU:HD12	1.97	0.45
2:D:94:LEU:HD12	2:D:105:LEU:HD22	1.97	0.45
1:A:80:ARG:O	1:A:84:GLY:N	2.49	0.45
1:B:94:VAL:HB	1:B:95:PRO:HD3	1.98	0.45
2:C:186:ILE:HG23	2:C:190:LEU:HD12	1.97	0.45
2:C:272:GLU:HG2	2:C:311:ILE:HG22	1.98	0.45
2:D:319:THR:HG22	2:D:320:GLN:N	2.32	0.45
1:A:85:THR:O	1:A:86:SER:CB	2.63	0.45
1:A:155:ILE:HG22	1:A:203:ILE:HD11	1.98	0.45
1:A:193:LEU:C	1:A:193:LEU:HD23	2.37	0.45
1:B:41:THR:CG2	1:B:52:LEU:HD21	2.46	0.45
1:B:59:ILE:O	1:B:62:ILE:HG22	2.17	0.45
2:C:8:THR:HG23	2:C:22:ASN:HA	1.97	0.45
1:A:72:LEU:C	1:A:72:LEU:HD23	2.37	0.45
2:D:37:ILE:CG2	2:D:213:VAL:HG22	2.47	0.45
2:D:208:CYS:O	2:D:225:VAL:HG21	2.17	0.45
2:D:220:ILE:HD12	2:D:234:THR:HG21	1.99	0.45
1:A:97:THR:C	1:A:99:GLY:H	2.18	0.44
2:C:62:VAL:CG1	2:C:69:LEU:HD12	2.48	0.44
2:D:99:VAL:HG11	2:D:141:LEU:HD21	1.99	0.44
2:C:103:VAL:HG21	2:C:125:LEU:CD1	2.44	0.44
1:A:85:THR:HG23	1:A:86:SER:N	2.32	0.44
1:A:163:MSE:O	1:B:163:MSE:CE	2.66	0.44
2:C:114:LYS:O	2:C:117:VAL:HG12	2.17	0.44
1:A:143:LEU:C	1:A:143:LEU:HD23	2.37	0.44
2:D:327:ILE:HG13	2:D:337:VAL:HG11	1.99	0.44
2:D:2:ILE:HG23	2:D:28:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:LEU:HD13	2:D:72:LEU:O	2.18	0.44
2:D:171:LEU:N	2:D:171:LEU:HD12	2.32	0.44
1:A:3:GLU:N	1:A:4:PRO:HD2	2.33	0.44
2:D:2:ILE:CG2	2:D:193:THR:HG21	2.48	0.44
2:D:234:THR:HG22	2:D:236:LEU:H	1.83	0.44
2:D:121:VAL:O	2:D:125:LEU:HD13	2.18	0.43
2:C:207:ILE:HG13	2:C:208:CYS:N	2.32	0.43
1:A:187:THR:O	1:A:188:VAL:CG1	2.61	0.43
1:B:85:THR:O	1:B:86:SER:CB	2.67	0.43
1:B:21:PHE:CD2	1:B:154:LEU:HD11	2.53	0.43
2:C:225:VAL:HG13	2:C:229:PHE:CE1	2.53	0.43
2:D:249:ILE:O	2:D:249:ILE:CD1	2.66	0.43
1:B:129:THR:HG23	1:B:131:MSE:H	1.83	0.43
2:C:18:ILE:N	2:C:18:ILE:HD12	2.34	0.43
2:D:2:ILE:HG21	2:D:193:THR:HG21	2.01	0.43
2:C:39:ALA:HB3	2:C:42:ALA:HB2	2.01	0.43
1:A:27:GLY:C	1:A:104:ILE:HD11	2.39	0.43
2:C:155:LEU:HD11	2:C:186:ILE:HD13	2.01	0.43
2:C:301:MSE:HG2	2:C:310:GLY:HA3	2.01	0.43
2:D:34:TYR:CD2	2:D:210:CYS:HB2	2.54	0.43
2:D:7:ILE:HG23	2:D:57:PRO:HB3	2.01	0.43
2:D:307:VAL:HG22	2:D:308:LYS:O	2.19	0.43
2:D:2:ILE:HG23	2:D:2:ILE:O	2.19	0.42
1:B:119:LEU:HD21	2:D:94:LEU:HD23	2.01	0.42
2:D:283:LEU:H	2:D:283:LEU:HD12	1.84	0.42
1:A:154:LEU:HD23	1:A:203:ILE:HD12	2.02	0.42
1:B:38:LEU:HD21	1:B:56:VAL:HG12	2.01	0.42
2:C:172:ASP:CG	2:C:175:THR:HG22	2.39	0.42
2:D:53:LEU:HD12	2:D:69:LEU:HB3	2.01	0.42
2:D:238:GLN:O	2:D:241:ILE:HG22	2.19	0.42
1:A:28:PHE:CD1	1:A:104:ILE:HD12	2.54	0.42
1:A:68:PHE:CZ	1:A:96:LEU:HD23	2.54	0.42
1:B:52:LEU:HD13	1:B:56:VAL:HG21	2.02	0.42
1:A:115:ILE:HD13	1:A:115:ILE:HG21	1.83	0.42
2:C:64:VAL:CG2	2:C:69:LEU:HD11	2.49	0.42
2:C:274:THR:HG21	2:C:334:HIS:HB3	2.01	0.42
2:C:327:ILE:HG23	2:C:337:VAL:HG11	2.02	0.42
1:B:85:THR:O	1:B:86:SER:HB3	2.19	0.42
2:D:195:LEU:HD13	2:D:196:LEU:N	2.35	0.42
1:A:193:LEU:O	1:A:197:VAL:HG23	2.20	0.41
2:C:21:LEU:HD21	2:C:47:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:LYS:O	2:D:197:ILE:HD13	2.20	0.41
2:D:165:ASP:OD1	2:D:197:ILE:HD11	2.20	0.41
2:D:270:ARG:HB2	2:D:340:LEU:HD11	2.02	0.41
1:A:12:GLY:C	1:A:172:LEU:HD13	2.41	0.41
1:A:126:MSE:SE	2:C:105:LEU:HD22	2.70	0.41
1:A:163:MSE:HG2	1:B:69:ILE:HB	2.01	0.41
1:B:142:ALA:O	1:B:146:LEU:HD13	2.21	0.41
2:D:211:VAL:HG13	2:D:228:VAL:HG21	2.02	0.41
2:D:307:VAL:HG22	2:D:308:LYS:N	2.34	0.41
1:A:1:MSE:HE3	1:A:5:MSE:HE3	2.02	0.41
2:D:2:ILE:HD12	2:D:161:VAL:CG1	2.51	0.41
1:A:85:THR:O	1:A:86:SER:OG	2.34	0.41
2:C:266:VAL:HG11	2:C:317:HIS:CG	2.56	0.41
1:A:147:VAL:HG11	1:A:210:ILE:HG23	2.02	0.41
2:D:168:THR:CB	2:D:176:THR:HG23	2.49	0.41
2:D:327:ILE:CG1	2:D:337:VAL:HG11	2.50	0.41
1:A:85:THR:CG2	1:A:91:ALA:HB2	2.51	0.41
2:C:214:ILE:O	2:C:214:ILE:HG23	2.21	0.41
2:D:234:THR:HB	2:D:237:ALA:CB	2.51	0.41
1:A:126:MSE:HE1	2:C:105:LEU:HD22	2.03	0.41
1:B:71:LEU:HD11	1:B:75:MSE:CE	2.51	0.41
2:C:103:VAL:CG2	2:C:125:LEU:HD11	2.46	0.41
2:C:301:MSE:HE1	2:C:312:MSE:HE3	2.02	0.41
2:D:60:GLY:O	2:D:70:THR:HG21	2.21	0.41
1:A:20:THR:HG21	1:A:158:VAL:HA	2.03	0.41
2:D:253:TYR:O	2:D:257:LEU:N	2.54	0.40
1:A:69:ILE:HG21	1:B:163:MSE:SE	2.70	0.40
1:A:123:SER:HA	1:A:126:MSE:CE	2.51	0.40
1:B:101:ALA:HB3	1:B:102:PRO:HD3	2.02	0.40
1:B:143:LEU:HG	1:B:214:VAL:HG21	2.02	0.40
2:D:146:LYS:O	2:D:149:VAL:HG22	2.21	0.40
1:A:131:MSE:HA	1:A:134:VAL:HG12	2.04	0.40
1:B:137:VAL:O	1:B:141:GLU:HB2	2.21	0.40
2:C:48:ILE:HG21	2:C:197:ILE:HD11	2.03	0.40
2:C:184:LYS:HG2	2:D:251:GLU:HG3	2.02	0.40
1:A:32:LEU:N	1:A:33:PRO:CD	2.85	0.40
1:B:6:MSE:O	1:B:10:VAL:HG23	2.21	0.40
2:D:196:LEU:N	2:D:196:LEU:HD13	2.36	0.40

There are no symmetry-related clashes.

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	214/217 (99%)	205 (96%)	6 (3%)	3 (1%)	9	40
1	B	213/217 (98%)	204 (96%)	9 (4%)	0	100	100
2	C	342/366 (93%)	318 (93%)	22 (6%)	2 (1%)	22	58
2	D	342/366 (93%)	324 (95%)	17 (5%)	1 (0%)	37	71
All	All	1111/1166 (95%)	1051 (95%)	54 (5%)	6 (0%)	25	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	VAL
1	A	188	VAL
2	C	132	ASP
2	C	133	LYS
1	A	47	ILE
2	D	2	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	170/162 (105%)	168 (99%)	2 (1%)	67	78
1	B	170/162 (105%)	168 (99%)	2 (1%)	67	78
2	C	299/311 (96%)	295 (99%)	4 (1%)	65	77
2	D	299/311 (96%)	292 (98%)	7 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	938/946 (99%)	923 (98%)	15 (2%)	58 74

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	188	VAL
1	B	106	ARG
1	B	163	MSE
2	C	102	ASN
2	C	253	TYR
2	C	269	LEU
2	C	307	VAL
2	D	6	ASN
2	D	52	ASN
2	D	196	LEU
2	D	249	ILE
2	D	283	LEU
2	D	322	ASP
2	D	334	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	187	ASN

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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	206/217 (94%)	-0.09	2 (0%) 79 65	118, 150, 193, 217	0
1	B	205/217 (94%)	-0.10	2 (0%) 79 65	124, 176, 223, 233	0
2	C	337/366 (92%)	0.07	5 (1%) 71 56	136, 176, 239, 290	0
2	D	337/366 (92%)	0.30	10 (2%) 52 39	124, 241, 289, 314	0
All	All	1085/1166 (93%)	0.08	19 (1%) 67 51	118, 178, 277, 314	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	294	ASN	3.2
1	B	85	THR	2.9
2	C	17	THR	2.8
2	D	154	ALA	2.8
2	D	130	LEU	2.7
2	D	242	GLN	2.6
1	A	216	ARG	2.5
2	C	294	ASN	2.5
2	D	161	VAL	2.5
2	D	121	VAL	2.4
2	D	150	ALA	2.4
2	C	137	TYR	2.3
2	C	283	LEU	2.3
2	D	103	VAL	2.2
1	B	89	LEU	2.1
2	C	154	ALA	2.1
2	D	241	ILE	2.1
2	D	143	GLY	2.1
1	A	187	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.