



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:56 AM EDT

PDB ID : 1VBF / pdb_00001vbf
Title : Crystal structure of protein L-isoaspartate O-methyltransferase homologue from *Sulfolobus tokodaii*
Authors : Tanaka, Y.; Tsumoto, K.; Yasutake, Y.; Umetsu, M.; Yao, M.; Tanaka, I.; Fukada, H.; Kumagai, I.
Deposited on : 2004-02-25
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

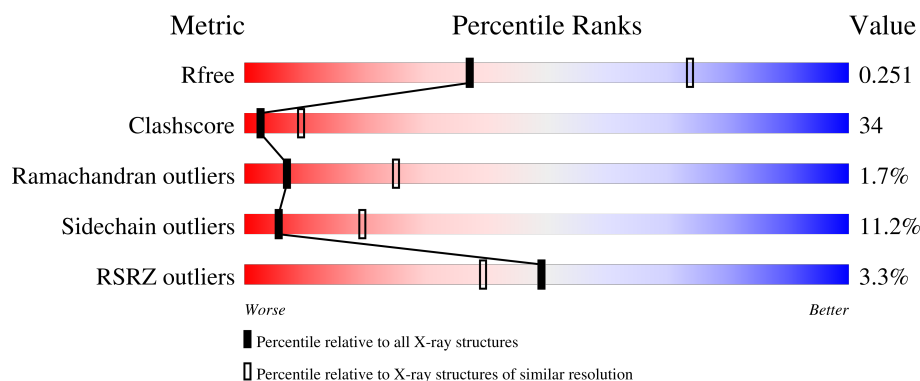
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

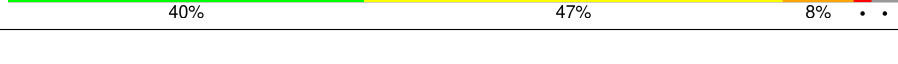
The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	
1	B	231	
1	C	231	
1	D	231	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7576 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 231aa long hypothetical protein-L-isoaspartate O-methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	Se	0	0	0
			1788	1159	288	336	1	4			
1	B	226	Total	C	N	O	S	Se	0	0	0
			1804	1167	291	341	1	4			
1	C	224	Total	C	N	O	S	Se	0	0	0
			1788	1159	288	336	1	4			
1	D	224	Total	C	N	O	S	Se	0	0	0
			1788	1159	288	336	1	4			

There are 20 discrepancies between the modelled and reference sequences:

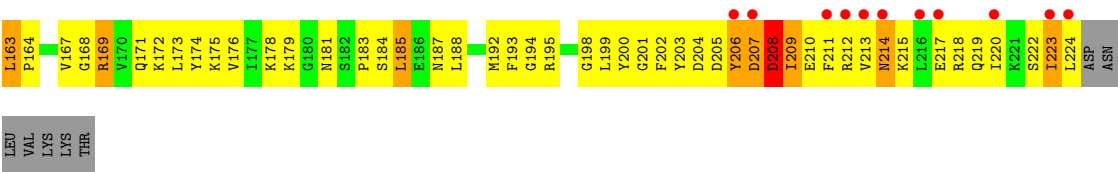
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	MET	SEE REMARK 999	UNP Q972K9
A	62	MSE	MET	modified residue	UNP Q972K9
A	104	MSE	MET	modified residue	UNP Q972K9
A	161	MSE	MET	modified residue	UNP Q972K9
A	192	MSE	MET	modified residue	UNP Q972K9
B	1	ALA	MET	SEE REMARK 999	UNP Q972K9
B	62	MSE	MET	modified residue	UNP Q972K9
B	104	MSE	MET	modified residue	UNP Q972K9
B	161	MSE	MET	modified residue	UNP Q972K9
B	192	MSE	MET	modified residue	UNP Q972K9
C	1	ALA	MET	SEE REMARK 999	UNP Q972K9
C	62	MSE	MET	modified residue	UNP Q972K9
C	104	MSE	MET	modified residue	UNP Q972K9
C	161	MSE	MET	modified residue	UNP Q972K9
C	192	MSE	MET	modified residue	UNP Q972K9
D	1	ALA	MET	SEE REMARK 999	UNP Q972K9
D	62	MSE	MET	modified residue	UNP Q972K9
D	104	MSE	MET	modified residue	UNP Q972K9
D	161	MSE	MET	modified residue	UNP Q972K9
D	192	MSE	MET	modified residue	UNP Q972K9

- Molecule 2 is water.

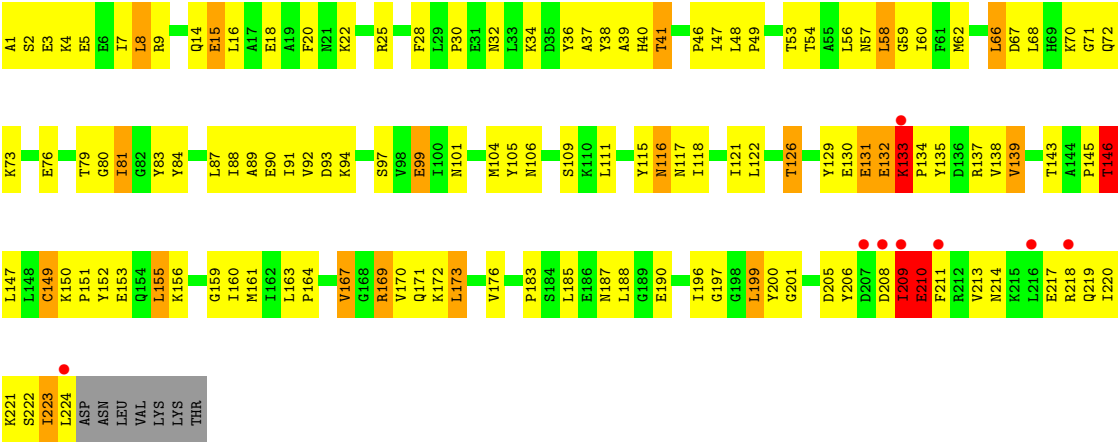
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total 90	O 90	0	0
2	B	140	Total 140	O 140	0	0
2	C	99	Total 99	O 99	0	0
2	D	79	Total 79	O 79	0	0

- Molecule 1: 231aa long hypothetical protein-L-isoaspartate O-methyltransferase





● Molecule 1: 231aa long hypothetical protein-L-isoaspartate O-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	277.80Å 277.80Å 277.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.3 (15.00-2.80) 99.3 (15.00-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.29 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.255 0.204 , 0.251	Depositor DCC
R_{free} test set	4310 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7576	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	0/1817	1.08	10/2447 (0.4%)
1	B	0.63	0/1833	1.17	13/2469 (0.5%)
1	C	0.62	0/1817	1.22	21/2447 (0.9%)
1	D	0.59	0/1817	1.09	10/2447 (0.4%)
All	All	0.60	0/7284	1.14	54/9810 (0.6%)

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	C	0	1

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	208	ASP	N-CA-C	19.12	138.48	109.41
1	B	225	ASP	N-CA-C	-10.27	100.87	113.50
1	C	207	ASP	N-CA-C	9.85	131.78	110.80
1	B	167	VAL	N-CA-C	-9.52	96.32	109.46
1	C	207	ASP	CA-C-N	-8.76	108.11	122.82
1	C	207	ASP	C-N-CA	-8.76	108.11	122.82
1	D	131	GLU	N-CA-C	7.93	120.92	111.33
1	B	22	LYS	N-CA-C	7.91	119.69	111.14
1	B	131	GLU	N-CA-C	7.38	121.94	112.34
1	C	44	ALA	N-CA-C	-7.13	101.12	110.53
1	C	156	LYS	N-CA-C	-6.97	101.54	110.53
1	C	133	LYS	N-CA-C	6.88	125.01	109.81
1	D	133	LYS	CA-C-N	-6.72	112.74	119.93
1	D	133	LYS	C-N-CA	-6.72	112.74	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	LYS	N-CA-C	6.55	124.29	109.81
1	C	205	ASP	N-CA-C	6.53	118.75	110.33
1	B	149	CYS	N-CA-C	6.37	117.89	111.07
1	A	144	ALA	CA-C-N	6.31	126.05	119.05
1	A	144	ALA	C-N-CA	6.31	126.05	119.05
1	B	51	ILE	N-CA-C	6.25	117.12	108.12
1	A	45	LEU	CA-C-N	6.24	127.21	119.98
1	A	45	LEU	C-N-CA	6.24	127.21	119.98
1	B	132	GLU	N-CA-C	-6.16	102.49	111.30
1	D	132	GLU	N-CA-C	-5.96	105.83	112.57
1	D	167	VAL	N-CA-C	-5.92	100.88	109.29
1	C	208	ASP	CA-C-N	5.83	132.46	121.97
1	C	208	ASP	C-N-CA	5.83	132.46	121.97
1	C	194	GLY	N-CA-C	-5.80	103.51	112.85
1	C	133	LYS	CA-C-N	-5.72	113.34	119.98
1	C	133	LYS	C-N-CA	-5.72	113.34	119.98
1	A	167	VAL	N-CA-C	-5.57	100.34	108.97
1	D	133	LYS	N-CA-C	5.53	122.04	109.81
1	C	174	TYR	N-CA-C	5.53	118.83	109.76
1	C	22	LYS	N-CA-C	5.53	118.14	111.40
1	B	184	SER	N-CA-C	-5.51	99.91	108.90
1	D	146	THR	CB-CA-C	-5.45	101.86	114.41
1	A	92	VAL	N-CA-C	5.42	117.52	109.17
1	B	71	GLY	N-CA-C	5.38	122.23	114.10
1	B	85	THR	N-CA-C	-5.38	105.33	111.14
1	B	194	GLY	N-CA-C	-5.38	105.39	112.82
1	D	149	CYS	N-CA-C	5.37	117.56	111.11
1	A	147	LEU	N-CA-C	-5.32	102.17	110.10
1	A	146	THR	CB-CA-C	-5.29	100.89	113.02
1	C	198	GLY	N-CA-C	5.20	118.62	112.33
1	A	133	LYS	N-CA-C	5.20	121.30	109.81
1	C	178	LYS	N-CA-C	5.16	117.79	110.10
1	C	23	VAL	N-CA-C	5.13	115.00	108.12
1	D	205	ASP	N-CA-C	5.10	117.11	110.53
1	C	73	LYS	N-CA-C	-5.10	100.09	108.41
1	C	157	GLU	N-CA-C	5.07	116.80	111.28
1	D	214	ASN	N-CA-C	-5.06	105.76	111.28
1	B	208	ASP	N-CA-C	-5.01	101.99	109.95
1	A	149	CYS	N-CA-C	5.00	117.12	111.02
1	C	132	GLU	N-CA-C	-5.00	104.66	111.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	114	TYR	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	1788	0	1830	93	0
1	B	1804	0	1840	126	0
1	C	1788	0	1830	137	0
1	D	1788	0	1830	156	0
2	A	90	0	0	4	0
2	B	140	0	0	8	0
2	C	99	0	0	7	0
2	D	79	0	0	11	0
All	All	7576	0	7330	490	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 34.

All (490) 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:B:126:THR:HG21	1:B:200:TYR:H	1.17	1.06
1:C:215:LYS:HG2	1:C:218:ARG:HH21	1.17	1.06
1:A:130:GLU:OE1	1:A:133:LYS:HD2	1.56	1.05
1:C:126:THR:HG21	1:C:200:TYR:H	1.23	1.00
1:C:155:LEU:HD22	1:C:159:GLY:HA3	1.47	0.97
1:A:126:THR:HG21	1:A:200:TYR:H	1.31	0.96
1:C:215:LYS:HG2	1:C:218:ARG:NH2	1.81	0.96
1:A:51:ILE:HG21	1:A:104:MSE:HE3	1.48	0.94
1:C:201:GLY:O	1:D:146:THR:HG23	1.71	0.90
1:D:176:VAL:HG22	1:D:185:LEU:HD22	1.53	0.89
1:A:146:THR:HG23	1:B:201:GLY:O	1.72	0.88
1:D:22:LYS:HD3	2:D:719:HOH:O	1.73	0.88
1:D:126:THR:HG21	1:D:200:TYR:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LEU:HD22	1:B:62:MSE:HE2	1.57	0.86
1:D:143:THR:HG21	1:D:171:GLN:CG	2.05	0.86
1:D:143:THR:HG21	1:D:171:GLN:HG2	1.56	0.86
1:C:68:LEU:HA	1:C:72:GLN:HE22	1.40	0.84
1:D:220:ILE:O	1:D:223:ILE:HG13	1.79	0.83
1:C:80:GLY:HA2	1:C:104:MSE:HE3	1.60	0.83
1:C:208:ASP:OD2	1:C:209:ILE:HD12	1.78	0.83
1:D:209:ILE:O	1:D:213:VAL:HG23	1.80	0.82
1:C:220:ILE:O	1:C:224:LEU:HB2	1.80	0.81
1:C:48:LEU:HD12	1:C:104:MSE:HG2	1.62	0.80
1:B:66:LEU:HD11	1:B:139:VAL:HG22	1.64	0.80
1:C:8:LEU:HD11	1:C:21:ASN:HD21	1.48	0.79
1:C:58:LEU:HD22	1:C:62:MSE:HE2	1.65	0.79
1:D:7:ILE:HD13	1:D:56:LEU:HD22	1.64	0.78
1:A:48:LEU:HD12	1:A:104:MSE:HE2	1.64	0.78
1:D:222:SER:C	1:D:224:LEU:H	1.89	0.77
1:A:126:THR:CG2	1:A:200:TYR:H	1.97	0.77
1:D:133:LYS:HB3	1:D:134:PRO:HD3	1.65	0.77
1:B:168:GLY:N	2:B:733:HOH:O	2.18	0.76
1:B:124:ASP:OD1	1:B:126:THR:HB	1.84	0.76
1:A:71:GLY:HA2	1:A:93:ASP:HB2	1.67	0.76
1:A:201:GLY:O	1:B:146:THR:HG23	1.86	0.76
1:C:66:LEU:HD11	1:C:139:VAL:HG22	1.68	0.75
1:B:149:CYS:O	1:B:153:GLU:HG3	1.86	0.75
1:C:167:VAL:HG13	1:C:195:ARG:NH2	2.02	0.75
1:C:203:TYR:CE1	1:D:146:THR:HG22	2.22	0.75
1:C:69:HIS:H	1:C:72:GLN:NE2	1.85	0.75
1:D:138:VAL:HG11	1:D:161:MSE:HE3	1.67	0.74
1:C:138:VAL:HG11	1:C:161:MSE:HE3	1.68	0.74
1:C:58:LEU:HD13	1:C:62:MSE:HE2	1.71	0.72
1:B:67:ASP:O	1:B:137:ARG:NH1	2.23	0.72
1:A:152:TYR:OH	1:A:183:PRO:HG3	1.90	0.72
1:B:7:ILE:HD11	1:B:41:THR:HG21	1.72	0.72
1:B:104:MSE:HE2	1:B:104:MSE:HA	1.70	0.71
1:B:169:ARG:HD2	2:B:569:HOH:O	1.91	0.71
1:B:138:VAL:HG11	1:B:161:MSE:HE3	1.73	0.70
1:D:152:TYR:OH	1:D:183:PRO:HG3	1.91	0.70
1:A:199:LEU:HD22	1:B:147:LEU:HD12	1.74	0.69
1:D:48:LEU:HD12	1:D:104:MSE:HG2	1.73	0.69
1:D:151:PRO:HB2	1:D:161:MSE:HE1	1.75	0.69
1:B:167:VAL:HB	2:B:733:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ILE:HD11	1:C:41:THR:CG2	2.22	0.69
1:A:150:LYS:HB2	1:A:151:PRO:HD3	1.75	0.69
1:B:126:THR:HG21	1:B:200:TYR:N	2.00	0.69
1:D:73:LYS:NZ	1:D:132:GLU:HB3	2.07	0.69
1:C:68:LEU:HA	1:C:72:GLN:NE2	2.07	0.69
1:C:208:ASP:HB2	1:C:209:ILE:CD1	2.23	0.69
1:C:215:LYS:O	1:C:218:ARG:HG2	1.93	0.69
1:D:5:GLU:O	1:D:9:ARG:HG2	1.93	0.69
1:D:72:GLN:O	1:D:92:VAL:HG13	1.93	0.69
1:B:220:ILE:O	1:B:224:LEU:HG	1.93	0.68
1:C:133:LYS:HB3	1:C:134:PRO:HD3	1.74	0.68
1:D:131:GLU:OE1	1:D:131:GLU:N	2.25	0.68
1:B:71:GLY:HA2	1:B:93:ASP:HB2	1.73	0.68
1:D:172:LYS:HD3	1:D:187:ASN:ND2	2.07	0.68
1:D:218:ARG:HG3	1:D:219:GLN:N	2.07	0.68
1:D:7:ILE:HD11	1:D:41:THR:CG2	2.23	0.68
1:D:58:LEU:HD13	1:D:62:MSE:HE2	1.76	0.68
1:B:62:MSE:HE1	1:B:193:PHE:HZ	1.59	0.68
1:D:66:LEU:HD11	1:D:139:VAL:HG13	1.76	0.68
1:A:84:TYR:O	1:A:88:ILE:HG13	1.93	0.67
1:D:14:GLN:NE2	1:D:15:GLU:H	1.92	0.67
1:D:41:THR:CG2	1:D:57:ASN:HB3	2.23	0.67
1:D:89:ALA:HB2	1:D:118:ILE:HD11	1.76	0.67
1:A:146:THR:CG2	1:B:201:GLY:O	2.42	0.67
1:B:72:GLN:HB2	1:B:92:VAL:HG22	1.77	0.67
1:C:167:VAL:HG13	1:C:195:ARG:HH21	1.59	0.67
1:D:14:GLN:HE21	1:D:15:GLU:HB2	1.60	0.67
1:A:56:LEU:HD22	1:A:60:ILE:HD13	1.76	0.67
1:B:126:THR:HG23	1:B:200:TYR:HB2	1.76	0.67
1:D:173:LEU:HD13	1:D:188:LEU:HD12	1.77	0.66
1:D:223:ILE:O	1:D:223:ILE:HG22	1.93	0.66
1:D:143:THR:HG22	1:D:164:PRO:HB2	1.77	0.66
1:A:200:TYR:C	1:B:146:THR:HG21	2.20	0.66
1:C:8:LEU:HD11	1:C:21:ASN:ND2	2.09	0.66
1:D:213:VAL:O	1:D:217:GLU:HG3	1.95	0.66
1:C:7:ILE:HD11	1:C:41:THR:HG21	1.76	0.66
1:A:184:SER:C	1:A:185:LEU:HD23	2.20	0.66
1:B:129:TYR:CZ	1:B:131:GLU:HG3	2.30	0.66
1:C:172:LYS:HG2	1:C:187:ASN:HD21	1.61	0.66
1:C:203:TYR:HE1	1:D:146:THR:HG22	1.60	0.66
1:A:71:GLY:CA	1:A:93:ASP:HB2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:LEU:N	1:C:185:LEU:HD23	2.11	0.66
1:D:53:THR:HG23	2:D:531:HOH:O	1.95	0.66
1:C:152:TYR:OH	1:C:183:PRO:HG3	1.96	0.65
1:B:24:ASP:HB3	1:B:27:LEU:HD22	1.77	0.65
1:B:66:LEU:O	1:B:137:ARG:HD2	1.96	0.65
1:A:220:ILE:HG22	1:A:220:ILE:O	1.97	0.65
1:A:5:GLU:O	1:A:9:ARG:HG3	1.97	0.65
1:C:58:LEU:HD13	1:C:62:MSE:CE	2.26	0.65
1:C:150:LYS:HB2	1:C:151:PRO:HD3	1.78	0.64
1:C:54:THR:HG21	1:C:62:MSE:HE1	1.78	0.64
1:A:220:ILE:O	1:A:220:ILE:CG2	2.45	0.64
1:A:167:VAL:HG13	1:A:195:ARG:NH2	2.14	0.63
1:C:56:LEU:CD2	1:C:60:ILE:HD13	2.27	0.63
1:A:176:VAL:HG22	1:A:185:LEU:HD22	1.79	0.63
1:C:200:TYR:C	1:D:146:THR:HG21	2.23	0.63
1:B:54:THR:HG21	1:B:62:MSE:CE	2.29	0.63
1:C:206:TYR:CG	1:C:207:ASP:N	2.65	0.63
1:C:167:VAL:HG12	1:C:168:GLY:N	2.13	0.63
1:C:72:GLN:O	1:C:92:VAL:HG13	1.98	0.63
1:B:113:SER:HA	2:B:633:HOH:O	1.98	0.62
1:B:66:LEU:HD22	1:B:137:ARG:HB3	1.81	0.62
1:C:126:THR:CG2	1:C:200:TYR:H	2.08	0.62
1:D:25:ARG:HH11	1:D:56:LEU:HD12	1.64	0.62
1:B:48:LEU:CD1	1:B:104:MSE:HE3	2.29	0.62
1:B:72:GLN:HB2	1:B:92:VAL:CG2	2.29	0.62
1:B:167:VAL:HG12	1:B:202:PHE:HE2	1.64	0.62
1:D:121:ILE:N	1:D:121:ILE:HD12	2.15	0.62
1:D:143:THR:O	1:D:196:ILE:HG22	2.00	0.62
1:B:223:ILE:C	1:B:225:ASP:H	2.06	0.62
1:D:7:ILE:HD11	1:D:41:THR:HG21	1.80	0.62
1:D:105:TYR:HA	2:D:510:HOH:O	1.99	0.62
1:A:126:THR:HG21	1:A:200:TYR:N	2.10	0.62
1:D:73:LYS:HG3	1:D:94:LYS:HG3	1.82	0.62
1:C:167:VAL:HG22	1:C:202:PHE:HE2	1.65	0.61
1:A:173:LEU:HD13	1:A:188:LEU:HD12	1.81	0.61
1:C:172:LYS:HD3	1:C:187:ASN:HD22	1.66	0.61
1:D:155:LEU:HD22	1:D:159:GLY:HA3	1.81	0.61
1:C:152:TYR:CZ	1:C:183:PRO:HG3	2.36	0.60
1:C:175:LYS:HB2	1:C:188:LEU:HD11	1.82	0.60
1:C:215:LYS:HA	1:C:218:ARG:HE	1.66	0.60
1:A:9:ARG:HH11	1:A:9:ARG:HG2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LYS:HB3	1:B:134:PRO:HD3	1.82	0.60
1:C:54:THR:HG21	1:C:62:MSE:CE	2.32	0.60
1:C:219:GLN:HG2	2:C:885:HOH:O	2.01	0.60
1:A:212:ARG:O	1:A:215:LYS:HG2	2.01	0.60
1:C:138:VAL:CG1	1:C:161:MSE:HE3	2.31	0.60
1:D:116:ASN:C	1:D:116:ASN:HD22	2.09	0.60
1:D:54:THR:HG21	1:D:62:MSE:HE1	1.83	0.60
1:B:48:LEU:HD12	1:B:104:MSE:HE3	1.83	0.60
1:D:170:VAL:HG11	1:D:190:GLU:OE1	2.02	0.60
1:D:71:GLY:HA2	1:D:93:ASP:HB2	1.83	0.60
1:B:143:THR:OG1	1:B:171:GLN:HG2	2.02	0.60
1:D:218:ARG:HG3	1:D:219:GLN:H	1.66	0.59
1:D:169:ARG:HG3	1:D:211:PHE:HZ	1.67	0.59
1:D:208:ASP:HB2	1:D:211:PHE:CE2	2.38	0.59
1:A:46:PRO:HA	1:A:52:ASN:ND2	2.17	0.59
1:D:4:LYS:HE2	1:D:38:TYR:CE2	2.37	0.59
1:D:143:THR:CG2	1:D:164:PRO:HB2	2.33	0.59
1:A:152:TYR:CZ	1:A:183:PRO:HG3	2.38	0.59
1:D:73:LYS:HZ1	1:D:132:GLU:HB3	1.67	0.59
1:D:83:TYR:CZ	1:D:87:LEU:HD11	2.38	0.59
1:C:214:ASN:O	1:C:217:GLU:HB2	2.03	0.59
1:D:89:ALA:CB	1:D:118:ILE:HD11	2.33	0.59
1:D:48:LEU:CD1	1:D:104:MSE:HG2	2.32	0.58
1:D:54:THR:HG21	1:D:62:MSE:CE	2.33	0.58
1:D:138:VAL:CG1	1:D:161:MSE:HE3	2.34	0.58
1:A:121:ILE:HG12	1:A:129:TYR:CE1	2.39	0.58
1:B:152:TYR:OH	1:B:183:PRO:HG3	2.04	0.58
1:D:208:ASP:HB2	1:D:211:PHE:HE2	1.68	0.58
1:B:67:ASP:HB3	1:B:137:ARG:NH1	2.18	0.58
1:B:150:LYS:HB2	1:B:151:PRO:HD3	1.85	0.58
1:B:54:THR:HG21	1:B:62:MSE:HE1	1.85	0.58
1:C:145:PRO:HG2	1:C:201:GLY:O	2.04	0.58
1:A:146:THR:HG21	1:B:200:TYR:C	2.29	0.57
1:A:208:ASP:O	1:A:212:ARG:HG3	2.04	0.57
1:C:80:GLY:HA2	1:C:104:MSE:CE	2.33	0.57
1:D:41:THR:HG22	1:D:57:ASN:HB3	1.86	0.57
1:B:73:LYS:HE2	1:B:132:GLU:HB3	1.86	0.57
1:D:1:ALA:O	1:D:2:SER:HB3	2.03	0.57
1:C:208:ASP:HB2	1:C:209:ILE:HD12	1.86	0.57
1:D:58:LEU:HD22	1:D:62:MSE:HE2	1.87	0.57
1:A:215:LYS:HG3	1:A:216:LEU:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:VAL:CG1	1:B:161:MSE:HE3	2.34	0.57
1:C:223:ILE:O	1:C:224:LEU:HG	2.05	0.57
1:B:119:LYS:HG2	1:B:121:ILE:CD1	2.35	0.57
1:C:167:VAL:HG21	1:D:167:VAL:HG21	1.86	0.57
1:C:147:LEU:HD23	1:C:148:LEU:N	2.20	0.57
1:B:146:THR:HG22	1:B:147:LEU:H	1.68	0.57
1:A:149:CYS:O	1:A:153:GLU:HG3	2.05	0.57
1:A:167:VAL:HG21	1:B:167:VAL:HG11	1.87	0.57
1:A:66:LEU:HD11	1:A:139:VAL:CG2	2.35	0.56
1:B:47:ILE:HG22	1:B:104:MSE:HE1	1.87	0.56
1:B:173:LEU:HD13	1:B:188:LEU:HD12	1.88	0.56
1:D:56:LEU:HD23	1:D:60:ILE:HD13	1.86	0.56
1:D:66:LEU:HD13	1:D:68:LEU:HD21	1.87	0.56
1:A:214:ASN:HB3	1:A:218:ARG:HH21	1.70	0.56
1:B:215:LYS:HA	1:B:218:ARG:NH1	2.21	0.56
1:D:41:THR:HG21	2:D:858:HOH:O	2.04	0.56
1:D:143:THR:HG21	1:D:171:GLN:CD	2.31	0.56
1:B:66:LEU:HD13	1:B:68:LEU:HD21	1.87	0.55
1:D:133:LYS:HB3	1:D:134:PRO:CD	2.34	0.55
1:B:176:VAL:HG22	1:B:185:LEU:HD22	1.88	0.55
1:D:219:GLN:O	1:D:222:SER:HB2	2.06	0.55
1:A:200:TYR:HA	1:B:146:THR:HG21	1.89	0.55
1:C:169:ARG:O	1:C:192:MSE:HG2	2.06	0.55
1:C:210:GLU:O	1:C:214:ASN:HB2	2.06	0.55
1:A:67:ASP:O	1:A:137:ARG:NH1	2.39	0.55
1:C:217:GLU:OE2	1:C:220:ILE:HD12	2.07	0.55
1:B:47:ILE:CG2	1:B:104:MSE:HE1	2.36	0.55
1:B:62:MSE:HE1	1:B:193:PHE:CZ	2.41	0.55
1:D:150:LYS:HB2	1:D:151:PRO:HD3	1.90	0.54
1:B:66:LEU:HD11	1:B:139:VAL:CG2	2.35	0.54
1:C:142:ALA:O	1:C:164:PRO:HD2	2.07	0.54
1:C:53:THR:HG23	2:C:528:HOH:O	2.07	0.54
1:A:71:GLY:C	1:A:93:ASP:HB2	2.33	0.54
1:C:201:GLY:O	1:D:146:THR:CG2	2.51	0.54
1:D:176:VAL:HG22	1:D:185:LEU:CD2	2.33	0.54
1:C:4:LYS:HE2	1:C:38:TYR:CE2	2.42	0.54
1:D:79:THR:HB	1:D:99:GLU:HG2	1.90	0.54
1:B:41:THR:HG22	1:B:57:ASN:HD22	1.73	0.54
1:B:66:LEU:CD2	1:B:137:ARG:HB3	2.38	0.54
1:C:56:LEU:HD23	1:C:60:ILE:HD13	1.89	0.54
1:D:46:PRO:O	1:D:47:ILE:HD13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLY:HA3	1:A:84:TYR:CE2	2.43	0.53
1:A:143:THR:OG1	1:A:171:GLN:HG2	2.07	0.53
1:B:119:LYS:HG2	1:B:121:ILE:HD11	1.91	0.53
1:C:112:LEU:HD12	1:C:120:LEU:HD11	1.91	0.53
1:C:206:TYR:CE2	1:C:207:ASP:HB3	2.44	0.53
1:C:208:ASP:O	1:C:212:ARG:HB2	2.08	0.53
1:D:222:SER:C	1:D:224:LEU:N	2.57	0.53
1:A:51:ILE:CG2	1:A:104:MSE:HE3	2.31	0.53
1:C:176:VAL:HG22	1:C:185:LEU:HD22	1.91	0.53
1:B:184:SER:C	1:B:185:LEU:HD23	2.34	0.53
1:A:215:LYS:CG	1:A:216:LEU:N	2.72	0.53
1:B:74:VAL:HG23	1:B:92:VAL:HG21	1.91	0.53
1:A:152:TYR:HH	1:A:183:PRO:HG3	1.74	0.52
1:C:69:HIS:O	1:C:72:GLN:HG3	2.09	0.52
1:B:62:MSE:HE3	1:B:141:TRP:HZ3	1.74	0.52
1:D:197:GLY:HA2	2:D:525:HOH:O	2.08	0.52
2:A:703:HOH:O	1:B:153:GLU:HG2	2.08	0.52
1:C:67:ASP:O	1:C:137:ARG:NH1	2.43	0.52
1:C:73:LYS:NZ	1:C:132:GLU:HB3	2.24	0.52
1:D:76:GLU:HG3	1:D:139:VAL:HG23	1.91	0.52
1:D:58:LEU:HD13	1:D:62:MSE:CE	2.40	0.52
1:D:72:GLN:O	1:D:92:VAL:CG1	2.57	0.52
1:D:81:ILE:HG22	1:D:83:TYR:H	1.74	0.52
1:B:218:ARG:HH11	1:B:218:ARG:HB2	1.74	0.52
1:C:200:TYR:HA	1:D:146:THR:HG21	1.90	0.52
1:D:169:ARG:CG	1:D:211:PHE:HZ	2.23	0.52
1:C:172:LYS:HD3	1:C:187:ASN:ND2	2.24	0.52
1:D:152:TYR:CZ	1:D:183:PRO:HG3	2.44	0.52
1:A:73:LYS:HD3	1:A:134:PRO:O	2.08	0.52
1:A:30:PRO:HB2	1:A:32:ASN:OD1	2.09	0.52
1:A:219:GLN:C	1:A:221:LYS:H	2.18	0.52
1:B:56:LEU:HD22	1:B:60:ILE:HG12	1.92	0.52
1:C:35:ASP:HB2	2:C:730:HOH:O	2.09	0.52
1:D:47:ILE:CD1	1:D:81:ILE:HD11	2.40	0.52
1:D:53:THR:OG1	1:D:81:ILE:HD12	2.10	0.52
1:D:169:ARG:CG	1:D:211:PHE:CZ	2.93	0.52
1:D:14:GLN:O	1:D:18:GLU:HG3	2.09	0.51
1:D:111:LEU:HB2	2:D:519:HOH:O	2.10	0.51
1:D:199:LEU:HD13	1:D:200:TYR:CE2	2.45	0.51
1:B:110:LYS:HD2	2:B:619:HOH:O	2.10	0.51
1:B:75:LEU:HB3	1:B:138:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LEU:O	1:B:138:VAL:HA	2.11	0.51
1:D:67:ASP:O	1:D:137:ARG:NH1	2.44	0.51
1:A:146:THR:HG22	1:B:203:TYR:CE1	2.46	0.50
1:C:62:MSE:HE1	1:C:193:PHE:HZ	1.75	0.50
1:B:126:THR:CG2	1:B:200:TYR:HD2	2.24	0.50
1:B:7:ILE:HD11	1:B:41:THR:CG2	2.39	0.50
1:A:66:LEU:HD13	1:A:68:LEU:HD21	1.92	0.50
1:A:133:LYS:HB3	1:A:134:PRO:HD3	1.92	0.50
1:B:30:PRO:HB2	1:B:32:ASN:OD1	2.10	0.50
1:C:151:PRO:HB2	1:C:161:MSE:HE1	1.93	0.50
1:C:211:PHE:N	1:C:211:PHE:CD2	2.77	0.50
1:D:66:LEU:CD1	1:D:139:VAL:HG13	2.40	0.50
1:D:92:VAL:CG1	1:D:93:ASP:N	2.75	0.50
1:B:206:TYR:HB2	1:B:211:PHE:CD2	2.47	0.50
1:C:155:LEU:HD22	1:C:159:GLY:CA	2.32	0.50
1:C:208:ASP:OD1	1:C:211:PHE:CE1	2.65	0.50
1:D:92:VAL:HG12	1:D:93:ASP:N	2.27	0.50
1:A:46:PRO:HA	1:A:52:ASN:HD22	1.75	0.50
1:B:157:GLU:O	1:B:178:LYS:HB3	2.12	0.49
1:D:15:GLU:HG3	2:D:776:HOH:O	2.13	0.49
1:D:53:THR:HG21	2:D:734:HOH:O	2.12	0.49
1:D:137:ARG:HD2	1:D:160:ILE:HB	1.94	0.49
1:B:167:VAL:HG12	1:B:202:PHE:CE2	2.46	0.49
1:C:209:ILE:O	1:C:213:VAL:HG23	2.13	0.49
1:A:2:SER:HB3	1:A:5:GLU:HB2	1.94	0.49
1:A:92:VAL:HG12	1:A:93:ASP:N	2.27	0.49
1:B:140:VAL:CG2	1:B:161:MSE:HE2	2.42	0.49
1:D:73:LYS:CE	1:D:132:GLU:HB3	2.43	0.49
1:D:7:ILE:CD1	1:D:56:LEU:HD22	2.38	0.49
1:D:169:ARG:HG3	1:D:211:PHE:CZ	2.46	0.49
1:D:223:ILE:O	1:D:223:ILE:CG2	2.59	0.49
1:B:140:VAL:HG21	1:B:161:MSE:HE2	1.94	0.49
1:C:172:LYS:CG	1:C:187:ASN:HD21	2.24	0.49
1:D:133:LYS:O	1:D:135:TYR:CD1	2.66	0.49
1:A:146:THR:HG22	1:B:203:TYR:HE1	1.78	0.49
1:D:209:ILE:HG23	1:D:210:GLU:H	1.77	0.49
1:B:205:ASP:CG	1:B:206:TYR:N	2.71	0.48
1:D:151:PRO:HB2	1:D:161:MSE:CE	2.41	0.48
1:A:7:ILE:HD11	1:A:41:THR:HB	1.94	0.48
1:B:41:THR:CG2	1:B:57:ASN:HD22	2.27	0.48
1:D:28:PHE:HB3	1:D:81:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LYS:O	1:D:134:PRO:C	2.55	0.48
1:A:200:TYR:CA	1:B:146:THR:HG21	2.44	0.48
1:D:3:GLU:OE1	1:D:41:THR:HB	2.14	0.48
1:B:53:THR:HG23	2:B:606:HOH:O	2.13	0.48
1:C:152:TYR:HH	1:C:183:PRO:HG3	1.79	0.48
1:A:213:VAL:O	1:A:214:ASN:C	2.56	0.48
1:D:173:LEU:CD1	1:D:188:LEU:HD12	2.43	0.48
1:A:45:LEU:HA	1:A:46:PRO:HD3	1.65	0.48
1:B:121:ILE:N	1:B:121:ILE:HD12	2.27	0.48
1:D:116:ASN:C	1:D:116:ASN:ND2	2.72	0.48
1:A:72:GLN:O	1:A:93:ASP:HB3	2.13	0.48
1:A:13:THR:HG22	1:A:16:LEU:H	1.79	0.48
1:A:215:LYS:HD2	2:A:892:HOH:O	2.14	0.48
1:B:169:ARG:H	1:B:169:ARG:HG2	1.30	0.47
1:A:155:LEU:HD22	1:A:159:GLY:HA3	1.95	0.47
1:B:175:LYS:HB2	1:B:188:LEU:HD11	1.96	0.47
1:A:51:ILE:HG21	1:A:104:MSE:CE	2.33	0.47
1:A:56:LEU:CD2	1:A:60:ILE:HD13	2.43	0.47
1:D:30:PRO:HB2	1:D:32:ASN:OD1	2.14	0.47
1:B:209:ILE:O	1:B:213:VAL:HG23	2.14	0.47
1:D:121:ILE:HG12	1:D:129:TYR:CE1	2.50	0.47
1:D:172:LYS:HD3	1:D:187:ASN:HD21	1.77	0.47
1:A:218:ARG:O	1:A:221:LYS:HB2	2.14	0.47
1:C:57:ASN:ND2	1:C:58:LEU:H	2.12	0.47
1:A:9:ARG:HG2	1:A:9:ARG:NH1	2.29	0.47
1:B:39:ALA:O	1:B:40:HIS:HB2	2.14	0.47
1:A:92:VAL:CG1	1:A:93:ASP:N	2.78	0.47
1:C:172:LYS:HD2	2:C:893:HOH:O	2.15	0.47
1:C:200:TYR:CA	1:D:146:THR:HG21	2.45	0.47
1:A:177:ILE:HB	1:A:184:SER:OG	2.15	0.47
1:B:181:ASN:C	1:B:183:PRO:HD3	2.40	0.47
1:C:25:ARG:NH1	1:C:56:LEU:HG	2.30	0.47
1:C:167:VAL:HG12	1:C:168:GLY:H	1.79	0.47
1:C:208:ASP:HB2	1:C:209:ILE:HG13	1.96	0.47
1:C:79:THR:HB	1:C:99:GLU:HG2	1.97	0.46
1:A:221:LYS:HA	1:A:221:LYS:HD3	1.56	0.46
1:B:169:ARG:NH1	1:B:208:ASP:OD2	2.48	0.46
1:A:129:TYR:CZ	1:A:131:GLU:HG3	2.49	0.46
1:B:110:LYS:H	1:B:110:LYS:HG2	1.31	0.46
1:B:172:LYS:HB2	1:B:172:LYS:HE3	1.65	0.46
1:A:4:LYS:HG3	1:A:38:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:LEU:CD2	1:C:62:MSE:HE2	2.39	0.46
1:A:120:LEU:HD22	2:A:769:HOH:O	2.14	0.46
1:B:223:ILE:C	1:B:225:ASP:N	2.74	0.46
1:A:72:GLN:O	1:A:92:VAL:CG1	2.64	0.46
1:C:67:ASP:HB3	1:C:137:ARG:NH1	2.30	0.46
1:D:84:TYR:O	1:D:88:ILE:HG13	2.15	0.46
1:B:62:MSE:CE	1:B:193:PHE:HZ	2.26	0.46
1:A:169:ARG:O	1:A:192:MSE:HG2	2.16	0.46
1:B:199:LEU:HD13	1:B:200:TYR:CE2	2.51	0.46
1:B:205:ASP:CG	1:B:206:TYR:H	2.24	0.46
1:C:58:LEU:CD1	1:C:62:MSE:HE2	2.43	0.46
1:C:130:GLU:HG2	1:C:133:LYS:HD2	1.98	0.46
1:D:137:ARG:CD	1:D:160:ILE:HB	2.46	0.46
1:D:170:VAL:CG1	1:D:190:GLU:HG3	2.46	0.46
1:B:169:ARG:NE	1:B:211:PHE:HE1	2.14	0.45
1:C:179:LYS:HD3	1:C:179:LYS:HA	1.54	0.45
1:C:211:PHE:O	1:C:215:LYS:HG3	2.15	0.45
1:D:7:ILE:HD11	1:D:41:THR:HG23	1.94	0.45
1:D:149:CYS:O	1:D:153:GLU:HG3	2.16	0.45
1:D:208:ASP:O	1:D:210:GLU:N	2.50	0.45
1:C:1:ALA:HB3	2:C:727:HOH:O	2.15	0.45
1:C:89:ALA:HB2	1:C:118:ILE:HD11	1.97	0.45
1:D:57:ASN:HB2	2:D:847:HOH:O	2.16	0.45
1:D:208:ASP:O	1:D:209:ILE:C	2.59	0.45
1:C:66:LEU:HD11	1:C:139:VAL:CG2	2.43	0.45
1:D:14:GLN:CG	1:D:15:GLU:N	2.80	0.45
1:B:126:THR:CG2	1:B:200:TYR:HB2	2.44	0.45
1:D:126:THR:CG2	1:D:200:TYR:H	2.19	0.45
1:B:92:VAL:HG13	1:B:93:ASP:N	2.31	0.45
1:B:94:LYS:HD3	1:C:114:TYR:CE1	2.52	0.45
1:C:7:ILE:HD11	1:C:41:THR:HG23	1.96	0.45
1:C:102:GLU:O	1:C:105:TYR:HB3	2.16	0.45
1:D:14:GLN:HG2	1:D:15:GLU:N	2.32	0.45
1:B:8:LEU:O	1:B:8:LEU:HD23	2.17	0.45
1:B:77:ILE:HB	1:B:140:VAL:HG13	1.99	0.45
1:D:70:LYS:HA	1:D:91:ILE:O	2.17	0.45
1:A:195:ARG:NH1	1:A:204:ASP:O	2.50	0.44
1:C:204:ASP:OD1	1:C:204:ASP:N	2.49	0.44
1:D:210:GLU:HB3	1:D:211:PHE:H	1.61	0.44
1:B:133:LYS:HB3	1:B:134:PRO:CD	2.47	0.44
1:B:155:LEU:HD22	1:B:159:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASP:CG	1:C:209:ILE:HD12	2.42	0.44
1:D:14:GLN:CD	1:D:15:GLU:H	2.24	0.44
1:D:221:LYS:O	1:D:221:LYS:HG2	2.16	0.44
1:C:206:TYR:CD2	1:C:207:ASP:HB2	2.53	0.44
1:A:199:LEU:CD2	1:B:147:LEU:HD12	2.47	0.44
1:D:66:LEU:HD22	1:D:137:ARG:HB3	1.99	0.44
1:D:156:LYS:HB3	2:D:759:HOH:O	2.18	0.44
1:C:181:ASN:C	1:C:183:PRO:HD3	2.43	0.44
1:A:201:GLY:O	1:B:146:THR:CG2	2.63	0.44
1:C:208:ASP:HB2	1:C:209:ILE:CG1	2.48	0.44
1:D:99:GLU:OE1	1:D:101:ASN:N	2.48	0.44
1:C:33:LEU:HD11	1:C:46:PRO:O	2.18	0.43
1:D:130:GLU:O	1:D:133:LYS:HB2	2.18	0.43
1:B:169:ARG:NE	1:B:211:PHE:CE1	2.87	0.43
1:C:155:LEU:CD2	1:C:159:GLY:HA3	2.32	0.43
1:C:41:THR:HG22	1:C:57:ASN:HB3	2.01	0.43
1:B:24:ASP:O	1:B:27:LEU:HB2	2.19	0.43
1:B:56:LEU:O	1:B:60:ILE:HG12	2.18	0.43
1:C:172:LYS:CD	1:C:187:ASN:ND2	2.82	0.43
1:C:211:PHE:HB3	2:C:797:HOH:O	2.17	0.43
1:B:46:PRO:HG3	2:B:813:HOH:O	2.19	0.43
1:C:32:ASN:ND2	1:C:33:LEU:HG	2.33	0.43
1:C:41:THR:CG2	1:C:57:ASN:HB3	2.48	0.43
1:C:213:VAL:O	1:C:214:ASN:C	2.61	0.43
1:B:58:LEU:O	1:B:62:MSE:HG3	2.18	0.43
1:B:121:ILE:CD1	1:B:121:ILE:N	2.82	0.43
1:C:83:TYR:CZ	1:C:87:LEU:HD11	2.54	0.43
1:C:119:LYS:HG2	1:C:121:ILE:CD1	2.49	0.43
1:D:39:ALA:O	1:D:40:HIS:HB2	2.19	0.43
1:A:112:LEU:HD13	1:A:120:LEU:HD21	2.01	0.42
1:B:114:TYR:O	1:B:114:TYR:CG	2.72	0.42
1:A:167:VAL:CG1	1:A:195:ARG:NH2	2.82	0.42
1:B:16:LEU:HA	1:B:91:ILE:HD11	2.00	0.42
1:B:127:LEU:HA	1:B:150:LYS:HG3	2.00	0.42
1:C:74:VAL:CG2	1:C:92:VAL:HG21	2.48	0.42
1:C:74:VAL:HG21	1:C:92:VAL:HG21	2.01	0.42
1:C:143:THR:OG1	1:C:171:GLN:HG2	2.19	0.42
1:C:167:VAL:CG1	1:C:168:GLY:N	2.81	0.42
1:A:122:LEU:HD22	1:A:122:LEU:C	2.45	0.42
1:C:66:LEU:O	1:C:137:ARG:HD2	2.19	0.42
1:D:170:VAL:HG13	1:D:190:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:OD1	1:A:126:THR:HB	2.19	0.42
1:B:74:VAL:CG2	1:B:92:VAL:HG21	2.49	0.42
1:D:30:PRO:O	1:D:34:LYS:HD2	2.19	0.42
1:A:35:ASP:HB2	2:A:702:HOH:O	2.17	0.42
1:A:74:VAL:HG22	1:A:137:ARG:HB2	2.02	0.42
1:A:184:SER:O	1:A:185:LEU:HD23	2.19	0.42
1:A:122:LEU:C	1:A:122:LEU:CD2	2.92	0.42
1:D:14:GLN:NE2	1:D:15:GLU:HB2	2.30	0.42
1:D:14:GLN:HE21	1:D:15:GLU:H	1.66	0.42
1:D:106:ASN:O	1:D:109:SER:HB3	2.20	0.42
1:B:70:LYS:HG3	2:B:575:HOH:O	2.19	0.42
1:D:37:ALA:C	1:D:38:TYR:CD1	2.98	0.42
1:D:73:LYS:HE3	1:D:94:LYS:CE	2.49	0.42
1:A:29:LEU:HA	1:A:30:PRO:HD3	1.94	0.42
1:A:87:LEU:O	1:A:91:ILE:HG13	2.20	0.42
1:B:54:THR:HG22	1:B:55:ALA:N	2.35	0.42
1:C:51:ILE:CG2	1:C:104:MSE:HE2	2.50	0.42
1:D:36:TYR:O	1:D:37:ALA:C	2.63	0.42
1:C:39:ALA:O	1:C:40:HIS:HB2	2.19	0.42
1:C:169:ARG:HD3	1:C:206:TYR:CE2	2.54	0.42
1:D:93:ASP:O	1:D:117:ASN:HB2	2.20	0.42
1:D:8:LEU:HD23	1:D:8:LEU:O	2.20	0.41
1:D:76:GLU:O	1:D:97:SER:HA	2.20	0.41
1:A:30:PRO:O	1:A:34:LYS:HG3	2.19	0.41
1:C:133:LYS:HB3	1:C:134:PRO:CD	2.49	0.41
1:D:133:LYS:CB	1:D:134:PRO:HD3	2.43	0.41
1:A:22:LYS:NZ	1:A:22:LYS:HB3	2.35	0.41
1:A:73:LYS:HE2	1:A:132:GLU:HB3	2.03	0.41
1:C:30:PRO:HB2	1:C:32:ASN:OD1	2.19	0.41
1:C:184:SER:C	1:C:185:LEU:HD23	2.45	0.41
1:C:209:ILE:HG13	1:C:209:ILE:H	1.34	0.41
1:C:222:SER:C	1:C:224:LEU:H	2.28	0.41
1:A:28:PHE:HA	1:A:111:LEU:HD13	2.01	0.41
1:B:84:TYR:O	1:B:88:ILE:HG13	2.19	0.41
1:C:66:LEU:HD22	1:C:137:ARG:HB3	2.03	0.41
1:C:163:LEU:HD12	1:C:163:LEU:H	1.85	0.41
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.90	0.41
1:D:59:GLY:HA2	1:D:62:MSE:HE3	2.02	0.41
1:B:130:GLU:O	1:B:133:LYS:HB2	2.21	0.41
1:C:124:ASP:OD1	1:C:126:THR:HB	2.20	0.41
1:D:172:LYS:HD3	1:D:187:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LEU:HD13	1:B:62:MSE:HE2	2.02	0.41
1:B:173:LEU:CD1	1:B:188:LEU:HD12	2.51	0.41
1:B:216:LEU:HD12	1:B:216:LEU:HA	1.89	0.41
1:C:48:LEU:CD1	1:C:104:MSE:HG2	2.41	0.41
1:C:151:PRO:CB	1:C:161:MSE:HE1	2.51	0.41
1:D:130:GLU:OE1	1:D:133:LYS:HD2	2.20	0.41
1:D:145:PRO:HG2	1:D:201:GLY:O	2.20	0.41
1:C:140:VAL:CG2	1:C:161:MSE:HE2	2.51	0.41
1:D:20:PHE:CE1	1:D:56:LEU:HD21	2.56	0.41
1:D:130:GLU:OE1	1:D:130:GLU:HA	2.21	0.41
1:D:80:GLY:HA2	1:D:104:MSE:HE3	2.03	0.40
1:D:90:GLU:OE2	1:D:115:TYR:CE1	2.74	0.40
1:B:215:LYS:HA	1:B:218:ARG:HH11	1.85	0.40
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.91	0.40
1:A:66:LEU:CD1	1:A:139:VAL:CG2	3.00	0.40
1:B:45:LEU:HA	1:B:46:PRO:HD3	1.72	0.40
1:C:46:PRO:O	1:C:47:ILE:HD13	2.21	0.40
1:C:66:LEU:CD1	1:C:139:VAL:HG22	2.44	0.40
1:D:209:ILE:HG23	1:D:210:GLU:N	2.36	0.40
1:D:210:GLU:O	1:D:213:VAL:N	2.51	0.40
1:B:99:GLU:O	1:B:122:LEU:HD23	2.22	0.40
1:B:169:ARG:HH11	1:B:169:ARG:HG3	1.86	0.40
1:D:53:THR:CG2	2:D:734:HOH:O	2.69	0.40
1:D:137:ARG:HD3	1:D:137:ARG:HA	1.85	0.40
1:B:66:LEU:CD1	1:B:139:VAL:HG22	2.43	0.40
1:C:2:SER:HB2	2:C:613:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/231 (96%)	206 (93%)	13 (6%)	3 (1%)	9	30
1	B	224/231 (97%)	208 (93%)	14 (6%)	2 (1%)	14	41
1	C	222/231 (96%)	201 (90%)	18 (8%)	3 (1%)	9	30
1	D	222/231 (96%)	204 (92%)	11 (5%)	7 (3%)	3	11
All	All	890/924 (96%)	819 (92%)	56 (6%)	15 (2%)	7	25

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	LYS
1	C	133	LYS
1	D	133	LYS
1	D	209	ILE
1	D	210	GLU
1	A	220	ILE
1	B	133	LYS
1	C	169	ARG
1	C	223	ILE
1	A	93	ASP
1	D	169	ARG
1	D	206	TYR
1	B	41	THR
1	D	223	ILE
1	D	49	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/196 (98%)	172 (89%)	21 (11%)	6	21
1	B	195/196 (100%)	173 (89%)	22 (11%)	5	19
1	C	193/196 (98%)	169 (88%)	24 (12%)	4	16
1	D	193/196 (98%)	173 (90%)	20 (10%)	7	22
All	All	774/784 (99%)	687 (89%)	87 (11%)	6	19

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	16	LEU
1	A	22	LYS
1	A	56	LEU
1	A	57	ASN
1	A	58	LEU
1	A	66	LEU
1	A	109	SER
1	A	122	LEU
1	A	126	THR
1	A	131	GLU
1	A	146	THR
1	A	147	LEU
1	A	163	LEU
1	A	169	ARG
1	A	173	LEU
1	A	199	LEU
1	A	204	ASP
1	A	210	GLU
1	A	219	GLN
1	A	220	ILE
1	B	16	LEU
1	B	21	ASN
1	B	27	LEU
1	B	41	THR
1	B	56	LEU
1	B	58	LEU
1	B	66	LEU
1	B	92	VAL
1	B	104	MSE
1	B	122	LEU
1	B	126	THR
1	B	131	GLU
1	B	139	VAL
1	B	146	THR
1	B	147	LEU
1	B	163	LEU
1	B	169	ARG
1	B	173	LEU
1	B	199	LEU
1	B	216	LEU
1	B	218	ARG

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Mol	Chain	Res	Type
1	B	223	ILE
1	C	5	GLU
1	C	8	LEU
1	C	16	LEU
1	C	21	ASN
1	C	56	LEU
1	C	57	ASN
1	C	58	LEU
1	C	66	LEU
1	C	99	GLU
1	C	104	MSE
1	C	122	LEU
1	C	126	THR
1	C	130	GLU
1	C	139	VAL
1	C	147	LEU
1	C	155	LEU
1	C	163	LEU
1	C	173	LEU
1	C	185	LEU
1	C	199	LEU
1	C	206	TYR
1	C	208	ASP
1	C	209	ILE
1	C	214	ASN
1	D	8	LEU
1	D	15	GLU
1	D	16	LEU
1	D	41	THR
1	D	58	LEU
1	D	66	LEU
1	D	81	ILE
1	D	99	GLU
1	D	116	ASN
1	D	122	LEU
1	D	126	THR
1	D	139	VAL
1	D	146	THR
1	D	147	LEU
1	D	155	LEU
1	D	163	LEU
1	D	173	LEU

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Mol	Chain	Res	Type
1	D	199	LEU
1	D	209	ILE
1	D	210	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	52	ASN
1	A	57	ASN
1	A	69	HIS
1	A	181	ASN
1	B	42	HIS
1	B	57	ASN
1	B	214	ASN
1	C	21	ASN
1	C	42	HIS
1	C	57	ASN
1	C	72	GLN
1	C	181	ASN
1	C	187	ASN
1	D	14	GLN
1	D	40	HIS
1	D	57	ASN
1	D	116	ASN
1	D	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	220/231 (95%)	-0.30	5 (2%) 61 51	26, 47, 70, 99	0
1	B	222/231 (96%)	-0.50	4 (1%) 67 58	23, 38, 58, 100	0
1	C	220/231 (95%)	-0.20	12 (5%) 30 23	28, 43, 97, 100	0
1	D	220/231 (95%)	-0.10	8 (3%) 46 37	31, 51, 87, 100	0
All	All	882/924 (95%)	-0.27	29 (3%) 49 39	23, 45, 83, 100	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	207	ASP	6.2
1	B	1	ALA	5.1
1	C	206	TYR	4.6
1	B	226	ASN	4.5
1	C	213	VAL	3.9
1	A	224	LEU	3.6
1	A	133	LYS	3.6
1	D	224	LEU	3.5
1	A	223	ILE	3.2
1	C	214	ASN	3.2
1	D	208	ASP	3.1
1	C	223	ILE	3.0
1	C	212	ARG	3.0
1	C	211	PHE	2.9
1	C	216	LEU	2.8
1	D	218	ARG	2.8
1	D	209	ILE	2.7
1	C	217	GLU	2.5
1	C	224	LEU	2.4
1	D	211	PHE	2.3
1	D	133	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	57	ASN	2.3
1	D	207	ASP	2.2
1	A	220	ILE	2.2
1	B	211	PHE	2.1
1	A	168	GLY	2.1
1	C	220	ILE	2.1
1	C	134	PRO	2.0
1	D	216	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.