



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:33 AM UTC

PDB ID : 5N6U / pdb_00005n6u
Title : Crystal structure of Beta-D-Mannosidase from Dictyoglomus thermophilum.
Authors : Richet, N.; Lafite, P.
Deposited on : 2017-02-16
Resolution : 3.08 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

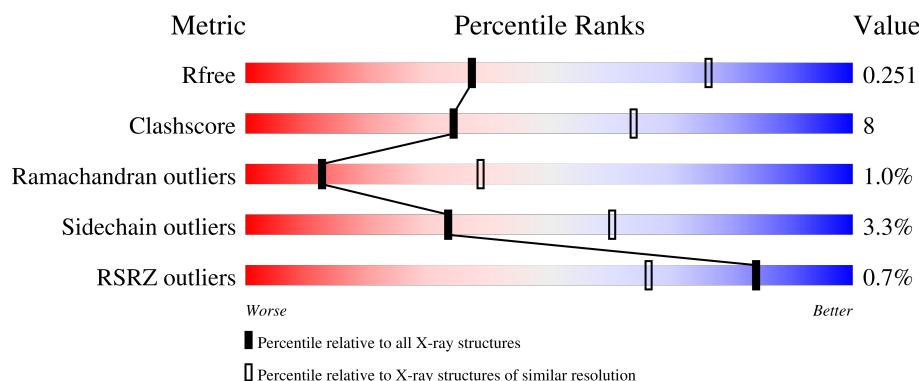
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	836	% 76% 18% ..
1	B	836	% 76% 18% ..
1	C	836	% 75% 20% ..
1	D	836	% 75% 19% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27265 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 Beta-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	811	Total	C	N	O	S	0	0	0
			6800	4431	1129	1224	16			
1	B	811	Total	C	N	O	S	0	0	0
			6800	4431	1129	1224	16			
1	C	811	Total	C	N	O	S	0	0	0
			6800	4431	1129	1224	16			
1	D	811	Total	C	N	O	S	0	0	0
			6800	4431	1129	1224	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP B5YAN4
A	-21	GLY	-	expression tag	UNP B5YAN4
A	-20	SER	-	expression tag	UNP B5YAN4
A	-19	SER	-	expression tag	UNP B5YAN4
A	-18	HIS	-	expression tag	UNP B5YAN4
A	-17	HIS	-	expression tag	UNP B5YAN4
A	-16	HIS	-	expression tag	UNP B5YAN4
A	-15	HIS	-	expression tag	UNP B5YAN4
A	-14	HIS	-	expression tag	UNP B5YAN4
A	-13	HIS	-	expression tag	UNP B5YAN4
A	-12	SER	-	expression tag	UNP B5YAN4
A	-11	SER	-	expression tag	UNP B5YAN4
A	-10	GLY	-	expression tag	UNP B5YAN4
A	-9	LEU	-	expression tag	UNP B5YAN4
A	-8	VAL	-	expression tag	UNP B5YAN4
A	-7	PRO	-	expression tag	UNP B5YAN4
A	-6	ARG	-	expression tag	UNP B5YAN4
A	-5	GLY	-	expression tag	UNP B5YAN4
A	-4	SER	-	expression tag	UNP B5YAN4
A	-3	HIS	-	expression tag	UNP B5YAN4
A	-2	MET	-	expression tag	UNP B5YAN4

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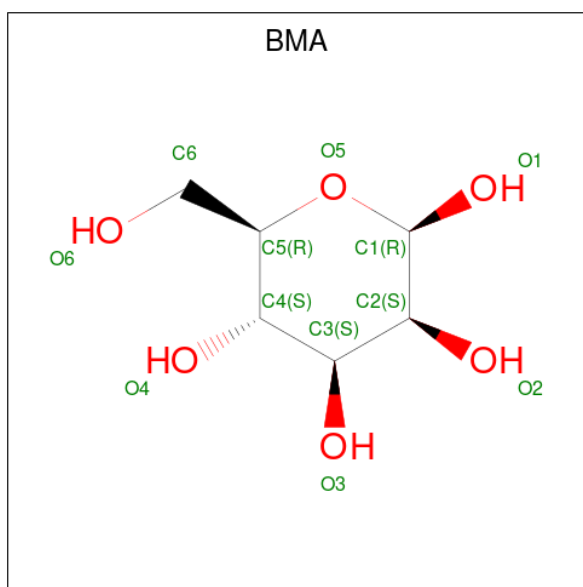
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP B5YAN4
A	0	SER	-	expression tag	UNP B5YAN4
A	425	CYS	GLU	engineered mutation	UNP B5YAN4
B	-22	MET	-	initiating methionine	UNP B5YAN4
B	-21	GLY	-	expression tag	UNP B5YAN4
B	-20	SER	-	expression tag	UNP B5YAN4
B	-19	SER	-	expression tag	UNP B5YAN4
B	-18	HIS	-	expression tag	UNP B5YAN4
B	-17	HIS	-	expression tag	UNP B5YAN4
B	-16	HIS	-	expression tag	UNP B5YAN4
B	-15	HIS	-	expression tag	UNP B5YAN4
B	-14	HIS	-	expression tag	UNP B5YAN4
B	-13	HIS	-	expression tag	UNP B5YAN4
B	-12	SER	-	expression tag	UNP B5YAN4
B	-11	SER	-	expression tag	UNP B5YAN4
B	-10	GLY	-	expression tag	UNP B5YAN4
B	-9	LEU	-	expression tag	UNP B5YAN4
B	-8	VAL	-	expression tag	UNP B5YAN4
B	-7	PRO	-	expression tag	UNP B5YAN4
B	-6	ARG	-	expression tag	UNP B5YAN4
B	-5	GLY	-	expression tag	UNP B5YAN4
B	-4	SER	-	expression tag	UNP B5YAN4
B	-3	HIS	-	expression tag	UNP B5YAN4
B	-2	MET	-	expression tag	UNP B5YAN4
B	-1	ALA	-	expression tag	UNP B5YAN4
B	0	SER	-	expression tag	UNP B5YAN4
B	425	CYS	GLU	engineered mutation	UNP B5YAN4
C	-22	MET	-	initiating methionine	UNP B5YAN4
C	-21	GLY	-	expression tag	UNP B5YAN4
C	-20	SER	-	expression tag	UNP B5YAN4
C	-19	SER	-	expression tag	UNP B5YAN4
C	-18	HIS	-	expression tag	UNP B5YAN4
C	-17	HIS	-	expression tag	UNP B5YAN4
C	-16	HIS	-	expression tag	UNP B5YAN4
C	-15	HIS	-	expression tag	UNP B5YAN4
C	-14	HIS	-	expression tag	UNP B5YAN4
C	-13	HIS	-	expression tag	UNP B5YAN4
C	-12	SER	-	expression tag	UNP B5YAN4
C	-11	SER	-	expression tag	UNP B5YAN4
C	-10	GLY	-	expression tag	UNP B5YAN4
C	-9	LEU	-	expression tag	UNP B5YAN4
C	-8	VAL	-	expression tag	UNP B5YAN4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	PRO	-	expression tag	UNP B5YAN4
C	-6	ARG	-	expression tag	UNP B5YAN4
C	-5	GLY	-	expression tag	UNP B5YAN4
C	-4	SER	-	expression tag	UNP B5YAN4
C	-3	HIS	-	expression tag	UNP B5YAN4
C	-2	MET	-	expression tag	UNP B5YAN4
C	-1	ALA	-	expression tag	UNP B5YAN4
C	0	SER	-	expression tag	UNP B5YAN4
C	425	CYS	GLU	engineered mutation	UNP B5YAN4
D	-22	MET	-	initiating methionine	UNP B5YAN4
D	-21	GLY	-	expression tag	UNP B5YAN4
D	-20	SER	-	expression tag	UNP B5YAN4
D	-19	SER	-	expression tag	UNP B5YAN4
D	-18	HIS	-	expression tag	UNP B5YAN4
D	-17	HIS	-	expression tag	UNP B5YAN4
D	-16	HIS	-	expression tag	UNP B5YAN4
D	-15	HIS	-	expression tag	UNP B5YAN4
D	-14	HIS	-	expression tag	UNP B5YAN4
D	-13	HIS	-	expression tag	UNP B5YAN4
D	-12	SER	-	expression tag	UNP B5YAN4
D	-11	SER	-	expression tag	UNP B5YAN4
D	-10	GLY	-	expression tag	UNP B5YAN4
D	-9	LEU	-	expression tag	UNP B5YAN4
D	-8	VAL	-	expression tag	UNP B5YAN4
D	-7	PRO	-	expression tag	UNP B5YAN4
D	-6	ARG	-	expression tag	UNP B5YAN4
D	-5	GLY	-	expression tag	UNP B5YAN4
D	-4	SER	-	expression tag	UNP B5YAN4
D	-3	HIS	-	expression tag	UNP B5YAN4
D	-2	MET	-	expression tag	UNP B5YAN4
D	-1	ALA	-	expression tag	UNP B5YAN4
D	0	SER	-	expression tag	UNP B5YAN4
D	425	CYS	GLU	engineered mutation	UNP B5YAN4

- Molecule 2 is beta-D-mannopyranose (CCD ID: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		

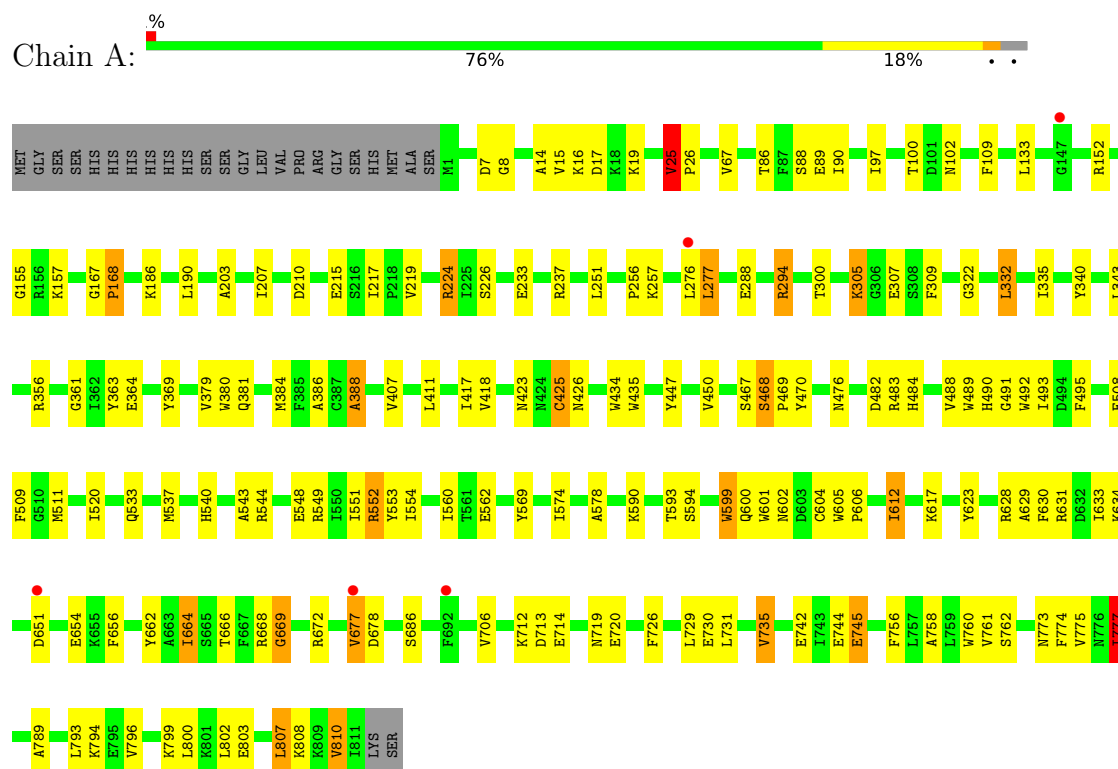
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	4	Total	O	0	0
			4	4		
3	C	10	Total	O	0	0
			10	10		
3	D	5	Total	O	0	0
			5	5		

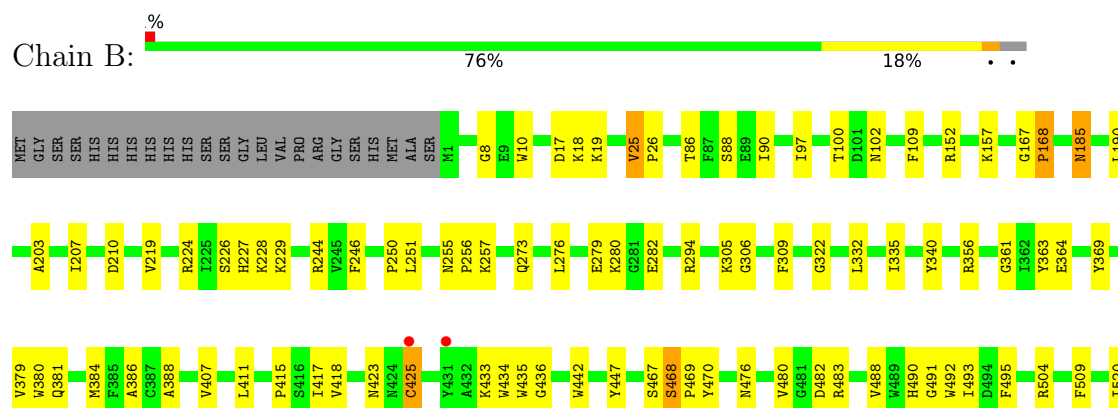
3 Residue-property plots [i](#)

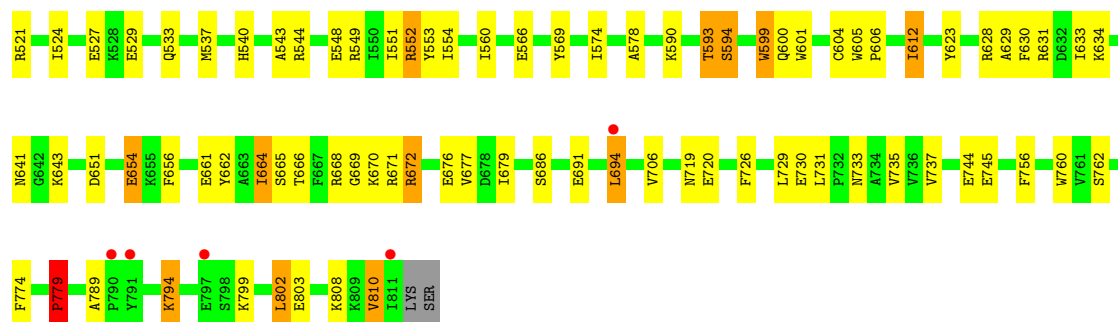
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Beta-mannosidase

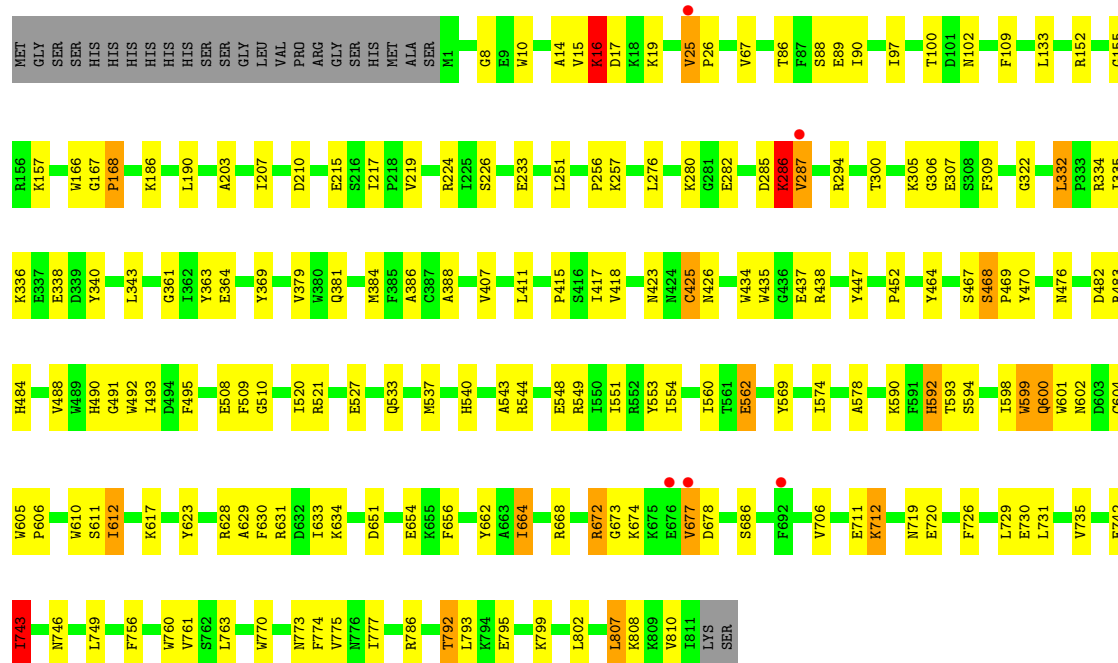
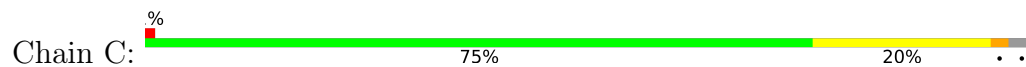


• Molecule 1: Beta-mannosidase

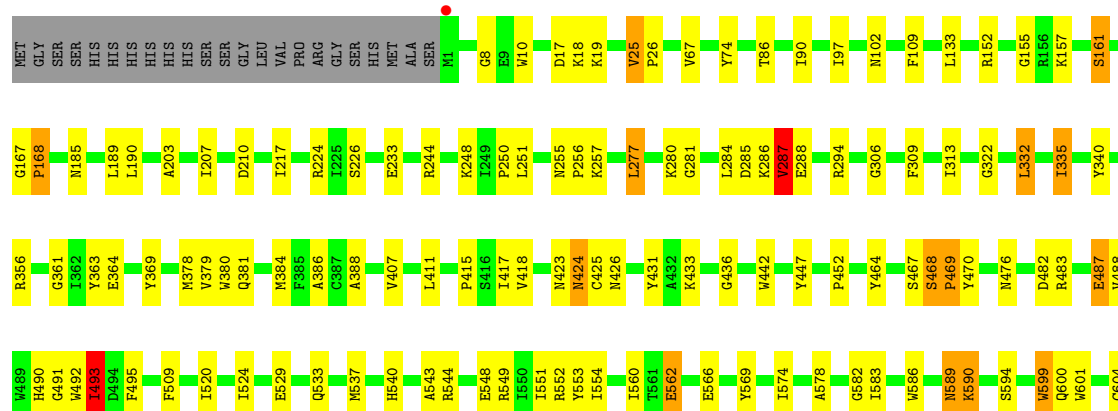
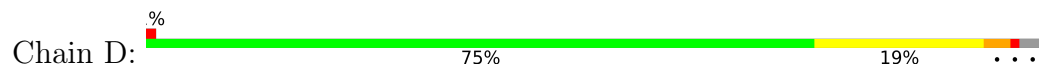


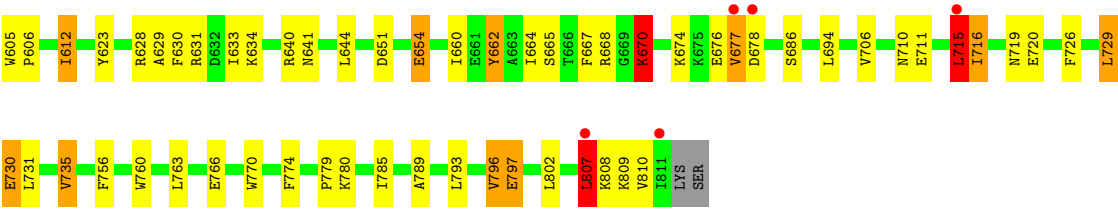


• Molecule 1: Beta-mannosidase



• Molecule 1: Beta-mannosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	139.25Å 75.56Å 217.88Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	49.50 – 3.08 49.50 – 3.19	Depositor EDS
% Data completeness (in resolution range)	88.2 (49.50-3.08) 98.8 (49.50-3.19)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.204 , 0.255 0.202 , 0.251	Depositor DCC
R_{free} test set	3775 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	81.8	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-l	Xtriage
Reported twinning fraction	0.913 for H, K, L 0.087 for -h,-k,l	Depositor
Outliers	4 of 75507 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27265	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.77	1/6995 (0.0%)	1.09	34/9461 (0.4%)
1	B	0.79	0/6995	1.10	31/9461 (0.3%)
1	C	0.80	7/6995 (0.1%)	1.10	30/9461 (0.3%)
1	D	0.81	5/6995 (0.1%)	1.14	46/9461 (0.5%)
All	All	0.79	13/27980 (0.0%)	1.11	141/37844 (0.4%)

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	7
1	B	0	7
1	C	0	4
1	D	0	6
All	All	0	24

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	711	GLU	CA-C	7.49	1.62	1.53
1	C	600	GLN	CA-C	-6.53	1.45	1.53
1	C	280	LYS	CA-C	6.10	1.57	1.52
1	C	807	LEU	CA-C	5.71	1.59	1.52
1	C	672	ARG	CA-C	5.39	1.59	1.53
1	C	25	VAL	CA-C	-5.32	1.47	1.52
1	D	670	LYS	N-CA	5.30	1.52	1.46
1	A	807	LEU	CA-C	5.30	1.59	1.52
1	C	712	LYS	N-CA	5.29	1.53	1.46
1	D	281	GLY	N-CA	5.28	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	287	VAL	CA-CB	5.11	1.59	1.54
1	D	590	LYS	CA-CB	-5.10	1.46	1.53
1	D	809	LYS	N-CA	5.03	1.52	1.45

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491	GLY	N-CA-C	-11.93	97.27	112.54
1	A	491	GLY	N-CA-C	-11.27	98.12	112.54
1	D	491	GLY	N-CA-C	-11.06	98.38	112.54
1	C	434	TRP	N-CA-C	11.05	124.64	111.82
1	D	715	LEU	CA-C-N	-10.97	104.84	120.42
1	D	715	LEU	C-N-CA	-10.97	104.84	120.42
1	B	672	ARG	N-CA-C	10.97	126.03	109.25
1	C	491	GLY	N-CA-C	-10.28	99.38	112.54
1	B	594	SER	N-CA-C	10.19	125.10	112.47
1	D	716	ILE	N-CA-C	-9.75	100.87	110.72
1	B	229	LYS	N-CA-C	-9.21	98.05	109.65
1	C	807	LEU	N-CA-C	9.17	124.00	109.50
1	A	807	LEU	N-CA-C	9.00	123.72	109.50
1	B	442	TRP	N-CA-C	8.81	123.58	113.01
1	D	716	ILE	N-CA-CB	8.50	123.33	110.58
1	D	442	TRP	N-CA-C	8.38	123.06	113.01
1	C	287	VAL	N-CA-C	-8.28	101.62	110.23
1	B	322	GLY	N-CA-C	8.09	122.91	111.19
1	D	807	LEU	N-CA-C	7.97	122.55	109.24
1	D	599	TRP	CA-C-N	-7.84	111.06	122.44
1	D	599	TRP	C-N-CA	-7.84	111.06	122.44
1	C	599	TRP	CA-CB-CG	-7.84	98.71	113.60
1	B	599	TRP	CA-C-N	-7.77	111.18	122.44
1	B	599	TRP	C-N-CA	-7.77	111.18	122.44
1	D	796	VAL	N-CA-CB	7.69	120.41	110.57
1	D	217	ILE	N-CA-C	7.65	115.46	109.19
1	A	599	TRP	CA-C-N	-7.60	111.43	122.44
1	A	599	TRP	C-N-CA	-7.60	111.43	122.44
1	D	589	ASN	CB-CA-C	-7.38	98.76	111.30
1	D	285	ASP	N-CA-C	-7.09	103.94	112.59
1	C	306	GLY	N-CA-C	7.07	124.18	111.02
1	D	322	GLY	N-CA-C	7.04	123.06	111.59
1	D	306	GLY	N-CA-C	7.02	124.08	111.02
1	B	593	THR	N-CA-C	6.97	121.91	113.41
1	A	305	LYS	N-CA-C	6.96	121.47	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	GLY	N-CA-C	6.92	122.87	111.59
1	A	810	VAL	CA-C-N	6.91	134.14	121.70
1	A	810	VAL	C-N-CA	6.91	134.14	121.70
1	C	322	GLY	N-CA-C	6.87	122.78	111.59
1	B	306	GLY	N-CA-C	6.84	123.75	111.02
1	A	714	GLU	N-CA-C	6.56	120.56	110.20
1	D	102	ASN	N-CA-C	6.50	120.19	108.48
1	D	662	TYR	CA-CB-CG	6.41	125.44	113.90
1	D	789	ALA	N-CA-C	6.39	116.36	108.11
1	B	794	LYS	CB-CG-CD	6.39	126.00	111.30
1	B	102	ASN	N-CA-C	6.38	119.96	108.48
1	B	679	ILE	N-CA-C	6.35	116.76	107.75
1	C	600	GLN	N-CA-C	6.33	119.18	107.60
1	D	674	LYS	N-CA-C	6.27	119.08	107.99
1	A	600	GLN	N-CA-C	6.20	118.53	107.80
1	A	102	ASN	N-CA-C	6.13	119.52	108.48
1	A	745	GLU	N-CA-CB	6.06	118.97	109.94
1	A	434	TRP	CB-CA-C	6.05	119.77	109.72
1	C	334	ARG	NE-CZ-NH2	-6.02	113.78	119.20
1	C	802	LEU	CA-CB-CG	5.96	137.17	116.30
1	A	288	GLU	N-CA-CB	5.96	120.12	110.41
1	C	102	ASN	N-CA-C	5.95	119.19	108.48
1	C	286	LYS	N-CA-C	-5.95	96.04	107.57
1	C	332	LEU	CA-C-N	-5.94	113.56	119.56
1	C	332	LEU	C-N-CA	-5.94	113.56	119.56
1	B	552	ARG	NE-CZ-NH2	5.94	124.54	119.20
1	C	600	GLN	CB-CA-C	-5.92	102.69	111.70
1	D	600	GLN	N-CA-C	5.89	117.99	107.80
1	B	794	LYS	N-CA-CB	5.88	119.28	110.22
1	D	633	ILE	CB-CA-C	-5.88	101.93	110.63
1	B	364	GLU	N-CA-C	5.87	117.62	110.41
1	C	388	ALA	N-CA-C	5.85	117.74	108.79
1	B	677	VAL	N-CA-C	5.84	118.36	109.12
1	C	282	GLU	N-CA-C	5.81	118.13	109.59
1	C	16	LYS	CB-CA-C	-5.77	103.86	111.82
1	A	288	GLU	N-CA-C	-5.72	101.22	110.32
1	B	388	ALA	N-CA-C	5.71	117.52	108.79
1	A	388	ALA	N-CA-C	5.68	117.48	108.79
1	D	386	ALA	N-CA-C	5.67	117.88	108.13
1	B	552	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	D	670	LYS	CA-CB-CG	5.66	125.42	114.10
1	D	487	GLU	N-CA-C	-5.65	104.33	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	599	TRP	N-CA-CB	5.64	120.35	110.42
1	B	600	GLN	N-CA-C	5.63	117.54	107.80
1	D	424	ASN	CB-CA-C	5.62	121.59	110.42
1	D	388	ALA	N-CA-C	5.59	117.35	108.79
1	A	712	LYS	CA-CB-CG	5.59	125.28	114.10
1	D	431	TYR	CB-CA-C	-5.56	101.40	110.85
1	D	425	CYS	N-CA-C	-5.52	105.23	112.41
1	D	288	GLU	N-CA-C	-5.52	100.69	109.96
1	B	694	LEU	N-CA-C	-5.51	104.00	111.55
1	D	640	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	D	277	LEU	N-CA-C	5.49	117.19	108.79
1	B	386	ALA	N-CA-C	5.49	117.57	108.13
1	B	737	VAL	CA-CB-CG1	5.49	119.73	110.40
1	A	599	TRP	N-CA-CB	5.47	119.32	110.40
1	D	281	GLY	N-CA-C	5.46	121.44	110.97
1	A	16	LYS	CB-CG-CD	5.44	123.81	111.30
1	C	438	ARG	N-CA-C	5.44	117.66	109.23
1	D	332	LEU	CA-C-N	-5.43	114.02	119.56
1	D	332	LEU	C-N-CA	-5.43	114.02	119.56
1	A	224	ARG	CB-CG-CD	5.42	123.78	111.30
1	D	364	GLU	N-CA-C	5.41	117.06	110.41
1	D	662	TYR	N-CA-CB	5.39	119.19	110.51
1	D	161	SER	N-CA-CB	5.38	118.50	110.22
1	B	789	ALA	N-CA-C	-5.36	99.98	108.82
1	C	25	VAL	CA-C-N	-5.35	113.15	119.84
1	C	25	VAL	C-N-CA	-5.35	113.15	119.84
1	B	425	CYS	N-CA-C	5.35	122.19	110.80
1	C	386	ALA	N-CA-C	5.33	117.30	108.13
1	C	364	GLU	N-CA-C	5.30	116.94	110.41
1	A	277	LEU	N-CA-C	5.29	116.88	108.79
1	C	285	ASP	N-CA-C	-5.26	100.66	109.24
1	A	789	ALA	N-CA-C	-5.26	100.14	108.82
1	C	673	GLY	N-CA-C	5.26	120.87	110.83
1	A	386	ALA	N-CA-C	5.25	117.15	108.13
1	D	67	VAL	N-CA-C	5.25	115.51	108.17
1	D	25	VAL	CA-C-N	-5.24	113.29	119.84
1	D	25	VAL	C-N-CA	-5.24	113.29	119.84
1	A	25	VAL	CA-C-N	-5.24	113.30	119.84
1	A	25	VAL	C-N-CA	-5.24	113.30	119.84
1	D	287	VAL	N-CA-C	5.24	114.14	106.55
1	D	599	TRP	N-CA-CB	5.23	118.93	110.40
1	D	566	GLU	N-CA-C	-5.21	105.24	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ASN	N-CA-CB	5.21	119.30	110.49
1	A	332	LEU	CA-C-N	-5.20	114.26	119.56
1	A	332	LEU	C-N-CA	-5.20	114.26	119.56
1	A	425	CYS	N-CA-C	5.18	121.83	110.80
1	C	67	VAL	N-CA-C	5.17	115.41	108.17
1	B	779	PRO	N-CA-C	5.14	123.06	112.47
1	B	566	GLU	N-CA-C	-5.11	105.35	111.03
1	A	777	ILE	CB-CA-C	5.11	118.02	110.77
1	A	294	ARG	CG-CD-NE	-5.10	100.77	112.00
1	D	161	SER	CA-CB-OG	5.10	121.30	111.10
1	D	729	LEU	CA-CB-CG	-5.10	98.45	116.30
1	A	450	VAL	CB-CA-C	-5.10	105.44	111.81
1	C	425	CYS	N-CA-C	5.09	121.65	110.80
1	B	599	TRP	N-CA-CB	5.09	118.69	110.40
1	A	67	VAL	N-CA-C	5.08	115.29	108.17
1	B	25	VAL	CA-C-N	-5.08	113.49	119.84
1	B	25	VAL	C-N-CA	-5.08	113.49	119.84
1	C	674	LYS	N-CA-C	5.07	116.58	108.41
1	A	364	GLU	N-CA-C	5.07	116.65	110.41
1	C	437	GLU	CA-C-O	-5.06	114.71	120.58
1	D	766	GLU	N-CA-C	5.06	118.22	111.75
1	A	435	TRP	N-CA-C	5.02	118.67	112.24

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	VAL	Peptide
1	A	257	LYS	Peptide
1	A	468	SER	Peptide
1	A	669	GLY	Peptide
1	A	713	ASP	Peptide
1	A	799	LYS	Peptide
1	A	807	LEU	Peptide
1	B	227	HIS	Mainchain,Peptide
1	B	228	LYS	Peptide
1	B	257	LYS	Peptide
1	B	468	SER	Peptide
1	B	671	ARG	Peptide
1	B	799	LYS	Peptide
1	C	257	LYS	Peptide
1	C	286	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	C	468	SER	Peptide
1	C	807	LEU	Peptide
1	D	257	LYS	Peptide
1	D	287	VAL	Peptide
1	D	468	SER	Peptide
1	D	670	LYS	Peptide
1	D	715	LEU	Peptide
1	D	807	LEU	Peptide

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	6800	0	6675	99	1
1	B	6800	0	6675	94	2
1	C	6800	0	6675	118	10
1	D	6800	0	6675	106	2
2	A	11	0	10	0	0
2	B	11	0	10	0	0
2	C	11	0	10	0	0
2	D	11	0	10	0	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
3	C	10	0	0	1	0
3	D	5	0	0	0	0
All	All	27265	0	26740	408	13

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (408) 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:C:305:LYS:HE2	1:C:592:HIS:CE1	1.85	1.11
1:B:590:LYS:NZ	1:B:651:ASP:OD1	2.01	0.94
1:A:590:LYS:NZ	1:A:651:ASP:OD1	2.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:GLN:HG3	1:C:610:TRP:O	1.66	0.94
1:D:590:LYS:NZ	1:D:651:ASP:OD1	2.02	0.93
1:C:590:LYS:NZ	1:C:651:ASP:OD1	2.01	0.92
1:C:10:TRP:CD1	1:C:25:VAL:HG22	2.07	0.89
1:B:10:TRP:CD1	1:B:25:VAL:HG22	2.08	0.88
1:A:388:ALA:O	1:A:426:ASN:ND2	2.07	0.88
1:B:643:LYS:NZ	1:B:691:GLU:OE2	2.06	0.87
1:D:10:TRP:CD1	1:D:25:VAL:HG22	2.10	0.86
1:C:743:ILE:HD11	1:C:749:LEU:HB2	1.61	0.81
1:B:488:VAL:O	1:B:553:TYR:OH	2.00	0.80
1:C:488:VAL:O	1:C:553:TYR:OH	2.00	0.80
1:C:305:LYS:HE2	1:C:592:HIS:ND1	1.97	0.80
1:D:715:LEU:O	1:D:716:ILE:C	2.24	0.79
1:A:488:VAL:O	1:A:553:TYR:OH	1.99	0.78
1:D:488:VAL:O	1:D:553:TYR:OH	2.00	0.78
1:C:166:TRP:NE1	1:C:599:TRP:HH2	1.82	0.78
1:A:599:TRP:O	1:A:599:TRP:CD2	2.38	0.76
1:C:599:TRP:CG	1:C:599:TRP:O	2.40	0.75
1:B:599:TRP:CD2	1:B:599:TRP:O	2.39	0.75
1:D:726:PHE:HA	1:D:729:LEU:HD12	1.68	0.75
1:D:694:LEU:HD12	1:D:694:LEU:O	1.88	0.74
1:C:305:LYS:CE	1:C:592:HIS:CE1	2.68	0.73
1:D:599:TRP:CD2	1:D:599:TRP:O	2.41	0.72
1:C:599:TRP:O	1:C:599:TRP:CD2	2.43	0.72
1:B:86:THR:CG2	1:B:157:LYS:HB3	2.21	0.71
1:B:599:TRP:O	1:B:599:TRP:CG	2.44	0.71
1:A:25:VAL:HG13	1:A:26:PRO:HD3	1.73	0.70
1:C:10:TRP:CD1	1:C:25:VAL:CG2	2.74	0.70
1:C:86:THR:CG2	1:C:157:LYS:HB3	2.22	0.70
1:A:86:THR:CG2	1:A:157:LYS:HB3	2.21	0.70
1:D:86:THR:CG2	1:D:157:LYS:HB3	2.21	0.69
1:A:224:ARG:HG2	1:A:233:GLU:HG2	1.73	0.69
1:C:604:CYS:HG	1:C:605:TRP:HD1	1.40	0.69
1:D:599:TRP:O	1:D:599:TRP:CG	2.45	0.69
1:A:599:TRP:O	1:A:599:TRP:CG	2.45	0.69
1:A:167:GLY:HA2	1:A:605:TRP:HE1	1.59	0.68
1:A:758:ALA:HB3	1:A:777:ILE:HG13	1.75	0.68
1:B:10:TRP:CD1	1:B:25:VAL:CG2	2.74	0.68
1:D:763:LEU:HD23	1:D:770:TRP:CZ3	2.28	0.68
1:B:665:SER:HB2	1:B:670:LYS:HA	1.75	0.68
1:C:332:LEU:O	1:C:335:ILE:HG12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:O	1:A:335:ILE:HG12	1.94	0.68
1:B:604:CYS:HG	1:B:605:TRP:HD1	1.40	0.68
1:D:10:TRP:CD1	1:D:25:VAL:CG2	2.76	0.68
1:D:715:LEU:CD1	1:D:785:ILE:HG22	2.25	0.67
1:A:88:SER:HG	1:A:100:THR:HG1	1.39	0.67
1:B:332:LEU:O	1:B:335:ILE:HG12	1.95	0.66
1:C:167:GLY:HA2	1:C:605:TRP:HE1	1.60	0.66
1:D:335:ILE:HD13	1:D:340:TYR:CE2	2.31	0.66
1:A:604:CYS:HG	1:A:605:TRP:HD1	1.43	0.66
1:C:598:ILE:HG22	1:C:600:GLN:H	1.60	0.66
1:B:167:GLY:HA2	1:B:605:TRP:HE1	1.61	0.65
1:C:763:LEU:HD23	1:C:770:TRP:CZ3	2.32	0.65
1:D:601:TRP:CZ3	1:D:612:ILE:HD11	2.31	0.65
1:C:601:TRP:CH2	1:C:612:ILE:HD11	2.32	0.64
1:C:761:VAL:CG2	1:C:777:ILE:HD11	2.28	0.64
1:D:644:LEU:HD13	1:D:694:LEU:HD21	1.78	0.64
1:D:167:GLY:HA2	1:D:605:TRP:HE1	1.61	0.64
1:B:733:ASN:HB3	1:B:808:LYS:HG3	1.77	0.64
1:C:601:TRP:CZ3	1:C:612:ILE:HD11	2.33	0.64
1:D:604:CYS:HG	1:D:605:TRP:HD1	1.45	0.63
1:B:661:GLU:HG2	1:B:676:GLU:HG2	1.81	0.63
1:B:601:TRP:CZ3	1:B:612:ILE:HD11	2.34	0.63
1:A:305:LYS:HG3	1:A:305:LYS:O	1.99	0.63
1:A:8:GLY:O	1:A:25:VAL:HG12	1.98	0.63
1:B:569:TYR:OH	1:B:760:TRP:HB2	1.99	0.62
1:C:86:THR:HG21	1:C:157:LYS:HD2	1.81	0.62
1:B:86:THR:HG21	1:B:157:LYS:HD2	1.80	0.62
1:D:424:ASN:O	1:D:469:PRO:HD2	1.99	0.62
1:A:601:TRP:CZ3	1:A:612:ILE:HD11	2.35	0.62
1:B:604:CYS:HG	1:B:605:TRP:CD1	2.18	0.62
1:D:369:TYR:OH	1:D:381:GLN:NE2	2.32	0.62
1:A:86:THR:HG21	1:A:157:LYS:HD2	1.79	0.62
1:D:86:THR:HG21	1:D:157:LYS:HB3	1.81	0.62
1:B:86:THR:HG21	1:B:157:LYS:HB3	1.81	0.62
1:D:601:TRP:CH2	1:D:612:ILE:HD11	2.35	0.62
1:C:305:LYS:O	1:C:305:LYS:HG3	1.99	0.61
1:A:86:THR:HG21	1:A:157:LYS:HB3	1.81	0.61
1:A:601:TRP:CH2	1:A:612:ILE:HD11	2.36	0.61
1:B:369:TYR:OH	1:B:381:GLN:NE2	2.33	0.61
1:C:224:ARG:HB3	1:C:233:GLU:HG2	1.82	0.61
1:B:601:TRP:CH2	1:B:612:ILE:HD11	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LEU:HD11	1:D:286:LYS:HB2	1.83	0.60
1:D:715:LEU:HD11	1:D:785:ILE:HG22	1.82	0.60
1:C:86:THR:HG21	1:C:157:LYS:HB3	1.81	0.60
1:C:604:CYS:HG	1:C:605:TRP:CD1	2.19	0.60
1:D:86:THR:HG21	1:D:157:LYS:HD2	1.81	0.60
1:B:794:LYS:O	1:B:794:LYS:HG2	2.00	0.60
1:D:294:ARG:HE	1:D:415:PRO:HA	1.66	0.60
1:D:332:LEU:O	1:D:335:ILE:HG13	2.01	0.60
1:B:305:LYS:O	1:B:305:LYS:HG3	2.01	0.60
1:C:369:TYR:OH	1:C:381:GLN:NE2	2.35	0.60
1:C:544:ARG:HG2	3:C:1005:HOH:O	2.02	0.59
1:C:25:VAL:HB	1:C:26:PRO:HD3	1.84	0.59
1:C:88:SER:HG	1:C:100:THR:HG1	1.44	0.59
1:C:773:ASN:OD1	1:C:774:PHE:N	2.36	0.59
1:A:369:TYR:OH	1:A:381:GLN:NE2	2.36	0.58
1:B:244:ARG:O	1:D:250:PRO:HG3	2.03	0.58
1:D:604:CYS:HG	1:D:605:TRP:CD1	2.22	0.58
1:D:361:GLY:C	1:D:384:MET:HE2	2.29	0.58
1:C:8:GLY:O	1:C:25:VAL:HG23	2.04	0.58
1:A:604:CYS:HG	1:A:605:TRP:CD1	2.22	0.58
1:B:25:VAL:HB	1:B:26:PRO:HD3	1.86	0.58
1:A:7:ASP:HA	1:A:25:VAL:HG11	1.86	0.57
1:B:8:GLY:O	1:B:25:VAL:HG23	2.04	0.57
1:C:664:ILE:HG23	1:C:672:ARG:HB3	1.85	0.57
1:A:664:ILE:HG23	1:A:672:ARG:HB3	1.85	0.57
1:C:361:GLY:C	1:C:384:MET:HE2	2.29	0.57
1:C:761:VAL:HG22	1:C:777:ILE:HD11	1.86	0.57
1:D:8:GLY:O	1:D:25:VAL:HG23	2.04	0.57
1:C:294:ARG:HE	1:C:415:PRO:HA	1.70	0.57
1:B:361:GLY:C	1:B:384:MET:HE2	2.30	0.56
1:B:17:ASP:OD2	1:B:19:LYS:NZ	2.37	0.56
1:C:343:LEU:HD23	1:C:602:ASN:HB3	1.87	0.56
1:B:664:ILE:HG23	1:B:672:ARG:HB2	1.86	0.56
1:D:25:VAL:HB	1:D:26:PRO:HD3	1.88	0.56
1:A:90:ILE:HD11	1:A:109:PHE:CE2	2.41	0.56
1:C:600:GLN:HB2	1:C:611:SER:HA	1.88	0.56
1:B:294:ARG:HE	1:B:415:PRO:HA	1.69	0.56
1:D:17:ASP:OD2	1:D:19:LYS:NZ	2.37	0.56
1:A:343:LEU:HD23	1:A:602:ASN:HB3	1.87	0.55
1:A:668:ARG:HG2	1:A:756:PHE:CD1	2.41	0.55
1:B:504:ARG:O	1:B:593:THR:O	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:LYS:O	1:C:287:VAL:C	2.48	0.55
1:D:90:ILE:HD11	1:D:109:PHE:CE2	2.42	0.55
1:A:773:ASN:OD1	1:A:774:PHE:N	2.36	0.55
1:C:17:ASP:OD2	1:C:19:LYS:NZ	2.39	0.55
1:C:668:ARG:HG2	1:C:756:PHE:CD1	2.41	0.55
1:A:8:GLY:N	1:A:25:VAL:CG1	2.70	0.55
1:B:90:ILE:HD11	1:B:109:PHE:CE2	2.42	0.55
1:C:590:LYS:O	1:C:593:THR:O	2.24	0.55
1:D:668:ARG:HG2	1:D:756:PHE:CD1	2.42	0.55
1:A:361:GLY:C	1:A:384:MET:HE2	2.32	0.55
1:B:88:SER:HG	1:B:100:THR:HG1	1.40	0.55
1:B:668:ARG:HG2	1:B:756:PHE:CD1	2.42	0.55
1:A:590:LYS:O	1:A:593:THR:O	2.25	0.55
1:C:90:ILE:HD11	1:C:109:PHE:CE2	2.42	0.55
1:D:424:ASN:O	1:D:468:SER:HB3	2.06	0.55
1:A:17:ASP:OD2	1:A:19:LYS:NZ	2.39	0.54
1:D:490:HIS:O	1:D:549:ARG:NH1	2.41	0.54
1:D:335:ILE:HD13	1:D:340:TYR:HE2	1.70	0.54
1:C:166:TRP:CD1	1:C:599:TRP:HH2	2.26	0.54
1:A:490:HIS:O	1:A:549:ARG:NH1	2.40	0.54
1:B:203:ALA:HB2	1:B:256:PRO:HG3	1.90	0.54
1:D:203:ALA:HB2	1:D:256:PRO:HG3	1.90	0.53
1:C:490:HIS:O	1:C:549:ARG:NH1	2.40	0.53
1:A:8:GLY:H	1:A:25:VAL:CG1	2.21	0.53
1:A:363:TYR:CZ	1:A:384:MET:HG2	2.44	0.53
1:B:363:TYR:CZ	1:B:384:MET:HG2	2.44	0.53
1:B:490:HIS:O	1:B:549:ARG:NH1	2.41	0.53
1:C:15:VAL:HG13	1:C:16:LYS:HD2	1.90	0.53
1:C:203:ALA:HB2	1:C:256:PRO:HG3	1.90	0.53
1:D:363:TYR:CZ	1:D:384:MET:HG2	2.44	0.53
1:B:733:ASN:CB	1:B:808:LYS:HG3	2.38	0.53
1:C:600:GLN:CG	1:C:610:TRP:O	2.49	0.53
1:D:224:ARG:HB3	1:D:233:GLU:HG3	1.90	0.53
1:D:488:VAL:HA	1:D:493:ILE:HG23	1.91	0.52
1:A:492:TRP:HE3	1:A:552:ARG:HD3	1.75	0.52
1:D:540:HIS:CD2	1:D:605:TRP:CZ3	2.97	0.52
1:C:735:VAL:HA	1:C:808:LYS:O	2.08	0.52
1:A:605:TRP:HB2	1:A:606:PRO:CD	2.40	0.52
1:A:726:PHE:HA	1:A:729:LEU:HD13	1.91	0.52
1:B:524:ILE:HD11	1:B:529:GLU:C	2.35	0.52
1:C:605:TRP:HB2	1:C:606:PRO:CD	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ALA:HB2	1:A:256:PRO:HG3	1.91	0.52
1:B:726:PHE:HA	1:B:729:LEU:HD13	1.91	0.52
1:C:363:TYR:CZ	1:C:384:MET:HG2	2.45	0.52
1:A:735:VAL:HA	1:A:808:LYS:O	2.10	0.51
1:D:487:GLU:O	1:D:493:ILE:CG2	2.58	0.51
1:A:742:GLU:OE1	1:A:794:LYS:HD2	2.11	0.51
1:C:726:PHE:HA	1:C:729:LEU:HD13	1.92	0.51
1:A:666:THR:HG1	1:A:669:GLY:H	1.59	0.51
1:A:677:VAL:HG12	1:A:678:ASP:H	1.76	0.50
1:C:540:HIS:CD2	1:C:605:TRP:CZ3	2.98	0.50
1:A:540:HIS:CD2	1:A:605:TRP:CZ3	3.00	0.50
1:C:562:GLU:HG2	1:D:562:GLU:HG2	1.92	0.50
1:D:284:LEU:CD1	1:D:286:LYS:HB2	2.42	0.50
1:B:630:PHE:O	1:B:631:ARG:C	2.54	0.50
1:D:677:VAL:HG12	1:D:678:ASP:H	1.76	0.50
1:C:677:VAL:HG12	1:C:678:ASP:H	1.76	0.50
1:D:509:PHE:O	1:D:599:TRP:N	2.45	0.50
1:B:629:ALA:HA	1:B:634:LYS:HE2	1.94	0.50
1:D:735:VAL:HA	1:D:808:LYS:O	2.12	0.50
1:C:749:LEU:HG	1:C:786:ARG:HG2	1.94	0.50
1:D:586:TRP:O	1:D:589:ASN:O	2.30	0.50
1:A:604:CYS:SG	1:A:605:TRP:HD1	2.35	0.49
1:D:411:LEU:HB3	1:D:417:ILE:CD1	2.42	0.49
1:D:730:GLU:HA	1:D:730:GLU:OE1	2.12	0.49
1:B:540:HIS:CD2	1:B:605:TRP:CZ3	3.00	0.49
1:B:628:ARG:NH2	1:B:774:PHE:O	2.44	0.49
1:C:423:ASN:HB3	1:C:447:TYR:CE1	2.47	0.49
1:C:509:PHE:O	1:C:599:TRP:N	2.44	0.49
1:C:742:GLU:HB2	1:C:793:LEU:CD1	2.42	0.49
1:B:604:CYS:SG	1:B:605:TRP:HD1	2.33	0.49
1:A:761:VAL:HG11	1:A:777:ILE:HD11	1.93	0.49
1:D:605:TRP:HB2	1:D:606:PRO:CD	2.42	0.49
1:A:423:ASN:HB3	1:A:447:TYR:CE1	2.48	0.49
1:B:623:TYR:C	1:B:623:TYR:CD1	2.90	0.49
1:D:604:CYS:SG	1:D:605:TRP:HD1	2.35	0.49
1:B:467:SER:HB3	1:B:470:TYR:HB2	1.95	0.49
1:B:605:TRP:HB2	1:B:606:PRO:CD	2.43	0.49
1:D:524:ILE:HD11	1:D:529:GLU:C	2.38	0.49
1:A:793:LEU:HD12	1:A:796:VAL:HG21	1.94	0.49
1:D:495:PHE:CD1	1:D:578:ALA:HA	2.48	0.48
1:C:335:ILE:HD12	1:C:340:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:ALA:HA	1:D:634:LYS:HE2	1.96	0.48
1:B:411:LEU:HB3	1:B:417:ILE:CD1	2.43	0.48
1:C:411:LEU:HB3	1:C:417:ILE:CD1	2.43	0.48
1:B:335:ILE:HD12	1:B:340:TYR:OH	2.13	0.48
1:B:551:ILE:O	1:B:554:ILE:HG22	2.14	0.48
1:C:294:ARG:O	1:C:294:ARG:HG3	2.13	0.48
1:D:644:LEU:HD13	1:D:694:LEU:CD2	2.43	0.48
1:B:294:ARG:O	1:B:294:ARG:HG3	2.12	0.48
1:C:604:CYS:SG	1:C:605:TRP:HD1	2.36	0.48
1:A:629:ALA:HA	1:A:634:LYS:HE2	1.95	0.48
1:B:495:PHE:CD1	1:B:578:ALA:HA	2.49	0.48
1:C:629:ALA:HA	1:C:634:LYS:HE2	1.95	0.48
1:A:628:ARG:NH2	1:A:774:PHE:O	2.47	0.48
1:C:224:ARG:CB	1:C:233:GLU:HG2	2.44	0.48
1:D:467:SER:HB3	1:D:470:TYR:HB2	1.96	0.48
1:D:423:ASN:HB3	1:D:447:TYR:CE1	2.48	0.48
1:D:551:ILE:O	1:D:554:ILE:HG22	2.13	0.48
1:D:807:LEU:O	1:D:808:LYS:HG2	2.14	0.48
1:C:305:LYS:CE	1:C:592:HIS:ND1	2.74	0.47
1:C:540:HIS:CD2	1:C:605:TRP:HZ3	2.33	0.47
1:C:495:PHE:CD1	1:C:578:ALA:HA	2.49	0.47
1:B:279:GLU:O	1:B:279:GLU:HG3	2.14	0.47
1:C:452:PRO:HG3	1:C:464:TYR:CE2	2.50	0.47
1:D:294:ARG:O	1:D:294:ARG:HG3	2.14	0.47
1:A:294:ARG:O	1:A:294:ARG:HG3	2.14	0.47
1:B:219:VAL:HG11	1:B:276:LEU:HD11	1.97	0.47
1:B:509:PHE:O	1:B:599:TRP:N	2.45	0.47
1:C:335:ILE:HD12	1:C:340:TYR:CZ	2.50	0.47
1:C:628:ARG:NH2	1:C:774:PHE:O	2.48	0.47
1:C:630:PHE:O	1:C:631:ARG:C	2.57	0.47
1:C:729:LEU:O	1:C:731:LEU:N	2.48	0.47
1:A:411:LEU:HB3	1:A:417:ILE:CD1	2.44	0.47
1:A:335:ILE:HD12	1:A:340:TYR:OH	2.14	0.47
1:C:215:GLU:HB2	1:C:217:ILE:HD11	1.97	0.47
1:D:74:TYR:CD1	1:D:185:ASN:OD1	2.68	0.47
1:A:492:TRP:CD1	1:B:492:TRP:HB2	2.50	0.47
1:C:14:ALA:O	1:C:15:VAL:C	2.58	0.47
1:D:628:ARG:NH2	1:D:774:PHE:O	2.48	0.47
1:D:630:PHE:O	1:D:631:ARG:C	2.58	0.47
1:A:335:ILE:HD12	1:A:340:TYR:CZ	2.50	0.46
1:A:630:PHE:O	1:A:631:ARG:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:VAL:HG11	1:C:276:LEU:HD11	1.96	0.46
1:A:219:VAL:HG11	1:A:276:LEU:HD11	1.97	0.46
1:A:551:ILE:O	1:A:554:ILE:HG22	2.15	0.46
1:B:335:ILE:HD12	1:B:340:TYR:CZ	2.50	0.46
1:B:423:ASN:HB3	1:B:447:TYR:CE1	2.49	0.46
1:C:508:GLU:CG	1:C:599:TRP:CD1	2.99	0.46
1:A:7:ASP:HA	1:A:25:VAL:CG1	2.44	0.46
1:A:509:PHE:O	1:A:599:TRP:N	2.45	0.46
1:B:794:LYS:O	1:B:794:LYS:CG	2.61	0.46
1:D:540:HIS:CD2	1:D:605:TRP:HZ3	2.34	0.46
1:C:520:ILE:HG23	1:C:537:MET:HE1	1.98	0.46
1:D:520:ILE:HG23	1:D:537:MET:HE1	1.97	0.46
1:C:467:SER:HB3	1:C:470:TYR:HB2	1.97	0.46
1:C:551:ILE:O	1:C:554:ILE:HG22	2.15	0.46
1:C:600:GLN:CG	1:C:600:GLN:O	2.60	0.46
1:A:666:THR:HG1	1:A:669:GLY:N	2.13	0.46
1:A:168:PRO:HD3	1:A:605:TRP:NE1	2.31	0.45
1:C:336:LYS:HG3	1:C:338:GLU:HB2	1.99	0.45
1:A:520:ILE:HG23	1:A:537:MET:HE1	1.98	0.45
1:A:729:LEU:O	1:A:731:LEU:N	2.49	0.45
1:D:726:PHE:CA	1:D:729:LEU:HD12	2.44	0.45
1:B:468:SER:O	1:B:482:ASP:OD2	2.34	0.45
1:C:166:TRP:NE1	1:C:599:TRP:CH2	2.73	0.45
1:C:510:GLY:HA2	1:C:600:GLN:HE22	1.82	0.45
1:C:633:ILE:CD1	1:C:656:PHE:CG	3.00	0.45
1:A:215:GLU:HB2	1:A:217:ILE:HD11	1.97	0.45
1:D:665:SER:HA	1:D:670:LYS:HB3	1.98	0.45
1:A:633:ILE:CD1	1:A:656:PHE:CG	3.00	0.45
1:A:495:PHE:CD1	1:A:578:ALA:HA	2.51	0.45
1:A:666:THR:OG1	1:A:669:GLY:N	2.45	0.45
1:A:476:ASN:O	1:A:483:ARG:NH1	2.49	0.45
1:B:670:LYS:HD3	1:B:779:PRO:HB2	1.98	0.45
1:C:168:PRO:HD3	1:C:605:TRP:NE1	2.32	0.45
1:D:667:PHE:HZ	1:D:729:LEU:HD22	1.81	0.45
1:A:309:PHE:O	1:A:594:SER:OG	2.35	0.45
1:A:468:SER:O	1:A:482:ASP:OD2	2.35	0.45
1:A:540:HIS:CD2	1:A:605:TRP:HZ3	2.35	0.45
1:C:468:SER:O	1:C:482:ASP:OD2	2.35	0.45
1:D:424:ASN:O	1:D:469:PRO:CD	2.64	0.45
1:C:166:TRP:CD1	1:C:599:TRP:CH2	3.05	0.45
1:C:476:ASN:O	1:C:483:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:SER:HB3	1:A:470:TYR:HB2	1.99	0.45
1:B:309:PHE:O	1:B:594:SER:OG	2.35	0.45
1:C:343:LEU:HD11	1:C:617:LYS:HG2	1.98	0.45
1:B:476:ASN:O	1:B:483:ARG:NH1	2.49	0.44
1:D:468:SER:O	1:D:482:ASP:OD2	2.35	0.44
1:D:569:TYR:OH	1:D:760:TRP:HB2	2.17	0.44
1:B:521:ARG:NH1	1:B:527:GLU:OE1	2.51	0.44
1:B:520:ILE:HG23	1:B:537:MET:HE1	1.99	0.44
1:B:729:LEU:O	1:B:731:LEU:N	2.50	0.44
1:B:744:GLU:O	1:B:745:GLU:C	2.61	0.44
1:C:309:PHE:O	1:C:594:SER:OG	2.35	0.44
1:D:309:PHE:O	1:D:594:SER:OG	2.35	0.44
1:A:569:TYR:OH	1:A:760:TRP:HB2	2.18	0.44
1:D:363:TYR:CE2	1:D:407:VAL:HG21	2.53	0.44
1:A:492:TRP:HB2	1:B:492:TRP:CD1	2.52	0.44
1:B:246:PHE:HB3	1:D:248:LYS:HB2	1.98	0.44
1:A:744:GLU:O	1:A:745:GLU:C	2.61	0.44
1:C:492:TRP:CD1	1:D:492:TRP:HB2	2.52	0.44
1:C:761:VAL:HG21	1:C:777:ILE:HD11	1.99	0.44
1:D:729:LEU:O	1:D:731:LEU:N	2.50	0.44
1:A:343:LEU:HD11	1:A:617:LYS:HG2	1.99	0.44
1:A:363:TYR:CE2	1:A:407:VAL:HG21	2.52	0.44
1:C:623:TYR:CD1	1:C:623:TYR:C	2.95	0.44
1:D:476:ASN:O	1:D:483:ARG:NH1	2.48	0.44
1:B:633:ILE:CD1	1:B:656:PHE:CG	3.01	0.43
1:D:710:ASN:HB2	1:D:716:ILE:HG21	1.99	0.43
1:A:623:TYR:CD1	1:A:623:TYR:C	2.96	0.43
1:B:168:PRO:HD3	1:B:605:TRP:NE1	2.32	0.43
1:D:543:ALA:O	1:D:544:ARG:C	2.61	0.43
1:C:363:TYR:CE2	1:C:407:VAL:HG21	2.53	0.43
1:C:569:TYR:OH	1:C:760:TRP:HB2	2.18	0.43
1:D:433:LYS:O	1:D:436:GLY:N	2.51	0.43
1:B:590:LYS:HB2	1:B:686:SER:HB3	2.00	0.43
1:D:582:GLY:O	1:D:583:ILE:C	2.61	0.43
1:C:15:VAL:HG13	1:C:16:LYS:HG3	1.99	0.43
1:B:250:PRO:HG3	1:D:244:ARG:O	2.19	0.43
1:C:492:TRP:HB2	1:D:492:TRP:CD1	2.54	0.43
1:B:224:ARG:NH1	1:B:273:GLN:OE1	2.52	0.43
1:D:668:ARG:HG2	1:D:756:PHE:CE1	2.54	0.43
1:B:540:HIS:CD2	1:B:605:TRP:HZ3	2.37	0.42
1:D:779:PRO:O	1:D:780:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:742:GLU:C	1:C:743:ILE:HD13	2.44	0.42
1:D:207:ILE:HD11	1:D:251:LEU:HD21	2.01	0.42
1:A:633:ILE:HD11	1:A:656:PHE:CD1	2.54	0.42
1:A:361:GLY:O	1:A:384:MET:HE2	2.20	0.42
1:A:590:LYS:HB2	1:A:686:SER:HB3	2.02	0.42
1:A:668:ARG:HG2	1:A:756:PHE:CE1	2.55	0.42
1:B:433:LYS:O	1:B:436:GLY:N	2.50	0.42
1:A:742:GLU:CD	1:A:794:LYS:HD2	2.44	0.42
1:C:207:ILE:HD11	1:C:251:LEU:HD21	2.00	0.42
1:D:294:ARG:HE	1:D:415:PRO:CA	2.32	0.42
1:C:508:GLU:HG2	1:C:599:TRP:CD1	2.54	0.42
1:D:487:GLU:O	1:D:493:ILE:HG22	2.20	0.42
1:D:623:TYR:CD1	1:D:623:TYR:C	2.97	0.42
1:C:426:ASN:ND2	1:C:447:TYR:OH	2.52	0.42
1:D:189:LEU:HD13	1:D:287:VAL:HG22	2.01	0.42
1:A:133:LEU:HD21	1:A:155:GLY:HA3	2.00	0.42
1:A:489:TRP:CZ2	1:A:549:ARG:HD2	2.55	0.42
1:B:361:GLY:O	1:B:384:MET:HE2	2.20	0.42
1:C:668:ARG:HG2	1:C:756:PHE:CE1	2.55	0.42
1:B:190:LEU:HB3	1:B:210:ASP:HB3	2.02	0.41
1:C:133:LEU:HD21	1:C:155:GLY:HA3	2.02	0.41
1:C:521:ARG:NH1	1:C:527:GLU:OE1	2.53	0.41
1:C:543:ALA:O	1:C:544:ARG:C	2.63	0.41
1:C:633:ILE:HD11	1:C:656:PHE:CD1	2.55	0.41
1:D:168:PRO:HD3	1:D:605:TRP:NE1	2.35	0.41
1:D:552:ARG:C	1:D:552:ARG:HD3	2.44	0.41
1:A:186:LYS:CD	1:A:217:ILE:HD13	2.50	0.41
1:C:361:GLY:O	1:C:384:MET:HE2	2.20	0.41
1:C:590:LYS:HB2	1:C:686:SER:HB3	2.02	0.41
1:B:207:ILE:HD11	1:B:251:LEU:HD21	2.03	0.41
1:B:356:ARG:HA	1:B:380:TRP:HB3	2.02	0.41
1:C:186:LYS:CD	1:C:217:ILE:HD13	2.50	0.41
1:A:552:ARG:HG3	1:A:552:ARG:HH11	1.85	0.41
1:B:335:ILE:HD12	1:B:340:TYR:CE2	2.56	0.41
1:B:363:TYR:CE2	1:B:407:VAL:HG21	2.54	0.41
1:B:434:TRP:HD1	1:B:435:TRP:CZ3	2.39	0.41
1:B:552:ARG:C	1:B:552:ARG:HD3	2.44	0.41
1:C:598:ILE:HG22	1:C:600:GLN:HG2	2.01	0.41
1:D:793:LEU:O	1:D:797:GLU:HG3	2.20	0.41
1:A:14:ALA:O	1:A:15:VAL:C	2.63	0.41
1:A:207:ILE:HD11	1:A:251:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:ARG:HG2	1:B:756:PHE:CE1	2.55	0.41
1:D:335:ILE:CD1	1:D:340:TYR:HE2	2.34	0.41
1:A:190:LEU:HB3	1:A:210:ASP:HB3	2.03	0.41
1:B:280:LYS:HD3	1:B:282:GLU:HB2	2.01	0.41
1:D:660:ILE:HG22	1:D:676:GLU:OE1	2.21	0.41
1:A:356:ARG:HA	1:A:380:TRP:HB3	2.03	0.41
1:A:543:ALA:O	1:A:544:ARG:C	2.63	0.41
1:A:552:ARG:HD2	1:B:492:TRP:CH2	2.56	0.41
1:B:590:LYS:HD2	1:B:590:LYS:HA	1.98	0.41
1:D:313:ILE:HD13	1:D:378:MET:HE1	2.03	0.41
1:D:590:LYS:HB2	1:D:686:SER:HB3	2.02	0.41
1:D:763:LEU:HB3	1:D:770:TRP:CZ2	2.56	0.41
1:D:807:LEU:HD12	1:D:807:LEU:C	2.46	0.41
1:A:484:HIS:CD2	1:A:508:GLU:HB2	2.56	0.41
1:C:598:ILE:CG2	1:C:600:GLN:HG2	2.51	0.41
1:C:792:THR:HG23	1:C:795:GLU:CB	2.51	0.41
1:D:426:ASN:ND2	1:D:447:TYR:OH	2.53	0.41
1:B:543:ALA:O	1:B:544:ARG:C	2.63	0.40
1:C:795:GLU:O	1:C:799:LYS:HB2	2.21	0.40
1:C:484:HIS:CD2	1:C:508:GLU:HB2	2.56	0.40
1:D:133:LEU:HD21	1:D:155:GLY:HA3	2.03	0.40
1:D:356:ARG:HA	1:D:380:TRP:HB3	2.02	0.40
1:D:452:PRO:HG3	1:D:464:TYR:CE1	2.57	0.40
1:A:762:SER:N	1:A:803:GLU:O	2.55	0.40
1:B:666:THR:OG1	1:B:669:GLY:N	2.46	0.40
1:B:762:SER:N	1:B:803:GLU:O	2.54	0.40
1:C:190:LEU:HB3	1:C:210:ASP:HB3	2.04	0.40
1:C:335:ILE:HD12	1:C:340:TYR:CE2	2.57	0.40
1:D:190:LEU:HB3	1:D:210:ASP:HB3	2.03	0.40
1:A:605:TRP:CD1	1:A:605:TRP:N	2.89	0.40
1:B:633:ILE:HD11	1:B:656:PHE:CD1	2.55	0.40
1:A:8:GLY:N	1:A:25:VAL:HG11	2.35	0.40
1:A:300:THR:OG1	1:A:307:GLU:OE1	2.39	0.40
1:A:511:MET:HE1	1:A:553:TYR:CE1	2.57	0.40
1:B:802:LEU:HD11	1:B:810:VAL:CG2	2.51	0.40
1:C:300:THR:OG1	1:C:307:GLU:OE1	2.39	0.40

All (13) 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:C:16:LYS:NZ	1:C:711:GLU:C[1_545]	0.73	1.47
1:C:16:LYS:CE	1:C:711:GLU:C[1_545]	1.10	1.10
1:C:16:LYS:NZ	1:C:712:LYS:N[1_545]	1.17	1.03
1:C:16:LYS:CE	1:C:711:GLU:O[1_545]	1.39	0.81
1:C:16:LYS:CE	1:C:712:LYS:N[1_545]	1.47	0.73
1:C:16:LYS:NZ	1:C:711:GLU:O[1_545]	1.51	0.69
1:C:16:LYS:CD	1:C:711:GLU:O[1_545]	1.91	0.29
1:D:18:LYS:NZ	1:D:654:GLU:OE1[1_565]	1.94	0.26
1:C:16:LYS:NZ	1:C:711:GLU:CA[1_545]	1.96	0.24
1:B:18:LYS:NZ	1:B:654:GLU:OE1[1_545]	2.12	0.08
1:C:16:LYS:CD	1:C:712:LYS:CA[1_545]	2.16	0.04
1:C:233:GLU:OE1	1:D:280:LYS:NZ[1_455]	2.16	0.04
1:A:237:ARG:NH2	1:B:279:GLU:OE2[1_455]	2.17	0.03

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	809/836 (97%)	723 (89%)	78 (10%)	8 (1%)	12	39
1	B	809/836 (97%)	715 (88%)	86 (11%)	8 (1%)	12	39
1	C	809/836 (97%)	723 (89%)	78 (10%)	8 (1%)	12	39
1	D	809/836 (97%)	725 (90%)	76 (9%)	8 (1%)	12	39
All	All	3236/3344 (97%)	2886 (89%)	318 (10%)	32 (1%)	12	39

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ARG
1	A	664	ILE
1	B	152	ARG
1	B	664	ILE
1	B	730	GLU

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Mol	Chain	Res	Type
1	C	152	ARG
1	C	664	ILE
1	D	152	ARG
1	D	664	ILE
1	D	730	GLU
1	A	730	GLU
1	C	730	GLU
1	B	641	ASN
1	D	641	ASN
1	A	469	PRO
1	B	469	PRO
1	B	779	PRO
1	C	469	PRO
1	D	469	PRO
1	A	800	LEU
1	B	168	PRO
1	C	168	PRO
1	A	168	PRO
1	A	677	VAL
1	C	677	VAL
1	D	168	PRO
1	D	677	VAL
1	A	493	ILE
1	B	493	ILE
1	C	493	ILE
1	D	493	ILE
1	C	743	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	727/748 (97%)	702 (97%)	25 (3%)	32	60
1	B	727/748 (97%)	705 (97%)	22 (3%)	36	62
1	C	727/748 (97%)	702 (97%)	25 (3%)	32	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	727/748 (97%)	702 (97%)	25 (3%)	32	60
All	All	2908/2992 (97%)	2811 (97%)	97 (3%)	33	60

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	89	GLU
1	A	97	ILE
1	A	226	SER
1	A	277	LEU
1	A	379	VAL
1	A	418	VAL
1	A	425	CYS
1	A	533	GLN
1	A	548	GLU
1	A	552	ARG
1	A	560	ILE
1	A	562	GLU
1	A	574	ILE
1	A	612	ILE
1	A	654	GLU
1	A	662	TYR
1	A	706	VAL
1	A	719	ASN
1	A	720	GLU
1	A	735	VAL
1	A	775	VAL
1	A	777	ILE
1	A	802	LEU
1	A	810	VAL
1	B	97	ILE
1	B	185	ASN
1	B	226	SER
1	B	255	ASN
1	B	379	VAL
1	B	418	VAL
1	B	425	CYS
1	B	480	VAL
1	B	533	GLN
1	B	548	GLU
1	B	560	ILE

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Mol	Chain	Res	Type
1	B	574	ILE
1	B	612	ILE
1	B	654	GLU
1	B	662	TYR
1	B	694	LEU
1	B	706	VAL
1	B	719	ASN
1	B	720	GLU
1	B	735	VAL
1	B	802	LEU
1	B	810	VAL
1	C	16	LYS
1	C	89	GLU
1	C	97	ILE
1	C	226	SER
1	C	379	VAL
1	C	418	VAL
1	C	425	CYS
1	C	435	TRP
1	C	533	GLN
1	C	548	GLU
1	C	560	ILE
1	C	562	GLU
1	C	574	ILE
1	C	592	HIS
1	C	612	ILE
1	C	654	GLU
1	C	662	TYR
1	C	706	VAL
1	C	719	ASN
1	C	720	GLU
1	C	743	ILE
1	C	746	ASN
1	C	775	VAL
1	C	792	THR
1	C	810	VAL
1	D	97	ILE
1	D	161	SER
1	D	226	SER
1	D	255	ASN
1	D	277	LEU
1	D	335	ILE

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Mol	Chain	Res	Type
1	D	379	VAL
1	D	418	VAL
1	D	493	ILE
1	D	533	GLN
1	D	548	GLU
1	D	560	ILE
1	D	562	GLU
1	D	574	ILE
1	D	612	ILE
1	D	654	GLU
1	D	662	TYR
1	D	706	VAL
1	D	719	ASN
1	D	720	GLU
1	D	735	VAL
1	D	796	VAL
1	D	797	GLU
1	D	802	LEU
1	D	810	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	36	ASN
1	A	93	ASN
1	A	202	ASN
1	A	214	GLN
1	A	227	HIS
1	A	314	ASN
1	A	381	GLN
1	A	413	ASN
1	A	426	ASN
1	A	478	GLN
1	A	502	ASN
1	A	540	HIS
1	A	565	ASN
1	A	589	ASN
1	A	751	ASN
1	B	30	HIS
1	B	36	ASN
1	B	202	ASN

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Mol	Chain	Res	Type
1	B	314	ASN
1	B	381	GLN
1	B	398	ASN
1	B	413	ASN
1	B	478	GLN
1	B	502	ASN
1	B	540	HIS
1	B	589	ASN
1	C	30	HIS
1	C	36	ASN
1	C	52	GLN
1	C	93	ASN
1	C	202	ASN
1	C	314	ASN
1	C	381	GLN
1	C	398	ASN
1	C	478	GLN
1	C	502	ASN
1	C	540	HIS
1	C	589	ASN
1	C	751	ASN
1	D	30	HIS
1	D	36	ASN
1	D	202	ASN
1	D	214	GLN
1	D	234	GLN
1	D	273	GLN
1	D	314	ASN
1	D	381	GLN
1	D	398	ASN
1	D	413	ASN
1	D	478	GLN
1	D	502	ASN
1	D	540	HIS
1	D	565	ASN
1	D	589	ASN
1	D	751	ASN

5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BMA	B	901	-	11,11,12	2.80	5 (45%)	15,15,17	1.92	2 (13%)
2	BMA	D	901	-	11,11,12	2.03	3 (27%)	15,15,17	1.64	2 (13%)
2	BMA	A	901	-	11,11,12	2.09	4 (36%)	15,15,17	1.37	3 (20%)
2	BMA	C	901	-	11,11,12	1.64	4 (36%)	15,15,17	1.36	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	B	901	-	-	2/2/19/22	0/1/1/1
2	BMA	D	901	-	-	0/2/19/22	0/1/1/1
2	BMA	A	901	-	-	2/2/19/22	0/1/1/1
2	BMA	C	901	-	-	2/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	BMA	O5-C1	6.66	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	BMA	C2-C3	4.43	1.59	1.52
2	D	901	BMA	C2-C3	4.24	1.59	1.52
2	B	901	BMA	C2-C3	3.82	1.58	1.52
2	D	901	BMA	O5-C1	3.55	1.49	1.43
2	B	901	BMA	O5-C5	3.48	1.50	1.43
2	A	901	BMA	O5-C1	3.19	1.49	1.43
2	C	901	BMA	O5-C1	2.72	1.48	1.43
2	B	901	BMA	C1-C2	2.55	1.58	1.52
2	D	901	BMA	O5-C5	2.44	1.48	1.43
2	C	901	BMA	C2-C3	2.41	1.56	1.52
2	C	901	BMA	O5-C5	2.26	1.47	1.43
2	A	901	BMA	O5-C5	2.23	1.47	1.43
2	A	901	BMA	C4-C3	2.16	1.57	1.52
2	C	901	BMA	C1-C2	2.05	1.57	1.52
2	B	901	BMA	C4-C3	2.02	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	BMA	O5-C5-C6	6.16	119.66	107.66
2	D	901	BMA	O5-C5-C6	3.83	115.12	107.66
2	A	901	BMA	C1-O5-C5	3.30	116.61	112.19
2	C	901	BMA	O6-C6-C5	-3.14	100.64	111.33
2	D	901	BMA	C1-O5-C5	2.92	116.10	112.19
2	A	901	BMA	O5-C5-C6	2.63	112.78	107.66
2	C	901	BMA	C1-O5-C5	2.42	115.43	112.19
2	A	901	BMA	C1-C2-C3	2.32	113.02	109.64
2	C	901	BMA	C1-C2-C3	2.23	112.89	109.64
2	B	901	BMA	C1-C2-C3	2.11	112.72	109.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	BMA	O5-C5-C6-O6
2	B	901	BMA	C4-C5-C6-O6
2	A	901	BMA	O5-C5-C6-O6
2	A	901	BMA	C4-C5-C6-O6
2	C	901	BMA	O5-C5-C6-O6
2	C	901	BMA	C4-C5-C6-O6

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	811/836 (97%)	-0.03	5 (0%)	85 69	45, 86, 130, 161	1 (0%)
1	B	811/836 (97%)	-0.05	7 (0%)	81 61	35, 81, 124, 160	1 (0%)
1	C	811/836 (97%)	-0.02	5 (0%)	85 69	41, 86, 127, 181	1 (0%)
1	D	811/836 (97%)	-0.05	6 (0%)	84 66	33, 82, 123, 175	1 (0%)
All	All	3244/3344 (97%)	-0.04	23 (0%)	84 66	33, 84, 126, 181	4 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	677	VAL	3.9
1	D	678	ASP	3.0
1	D	715	LEU	2.9
1	C	677	VAL	2.9
1	C	287	VAL	2.7
1	D	807	LEU	2.7
1	B	694	LEU	2.6
1	B	811	ILE	2.5
1	B	797	GLU	2.5
1	B	431	TYR	2.4
1	D	811	ILE	2.4
1	B	790	PRO	2.2
1	B	425	CYS	2.2
1	A	651	ASP	2.2
1	A	147	GLY	2.2
1	D	677	VAL	2.2
1	C	676	GLU	2.1
1	A	276	LEU	2.1
1	C	692	PHE	2.1
1	D	1	MET	2.0
1	A	692	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	25	VAL	2.0
1	B	791	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	C	901	11/12	0.86	0.17	87,103,115,116	0
2	BMA	B	901	11/12	0.87	0.14	58,69,79,82	0
2	BMA	A	901	11/12	0.92	0.13	71,87,95,98	0
2	BMA	D	901	11/12	0.92	0.13	75,94,105,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.