



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:17 PM GMT

PDB ID : 1WZX  
Title : Crystal Structure of Family 30 Carbohydrate Binding Module.  
Authors : Horiguchi, Y.; Kono, M.; Suzuki, A.; Yamane, T.; Arai, M.; Sakka, K.; Omiya, K.  
Deposited on : 2005-03-10  
Resolution : 3.52 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

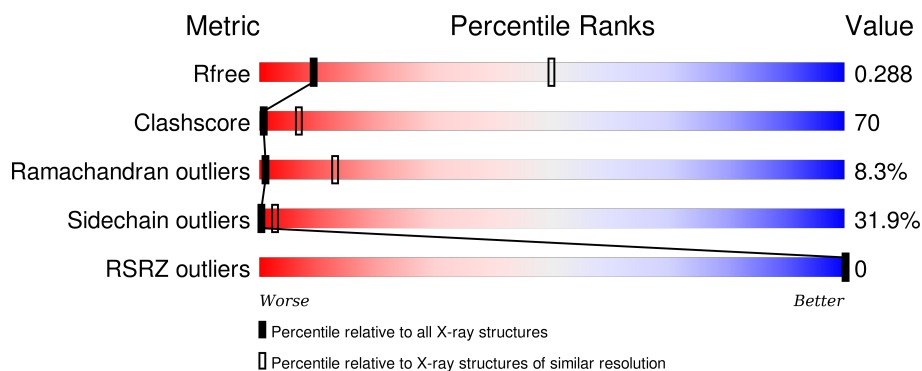
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.52 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))
$R_{free}$	91344	1089 (3.64-3.40)
Clashscore	102246	1197 (3.64-3.40)
Ramachandran outliers	100387	1159 (3.64-3.40)
Sidechain outliers	100360	1160 (3.64-3.40)
RSRZ outliers	91569	1096 (3.64-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	205	
1	B	205	
1	C	205	
1	D	205	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5564 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.

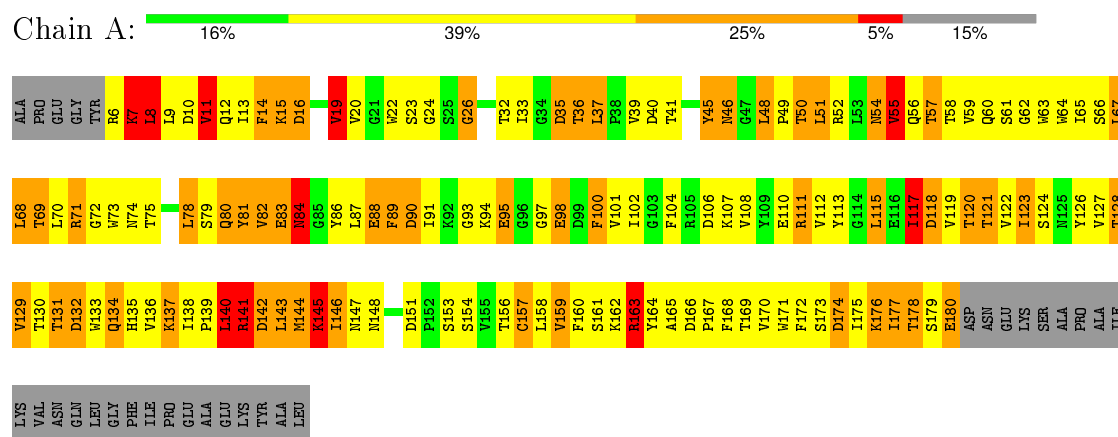
- Molecule 1 is a protein called COG3291: FOG: PKD repeat.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1404	904	227	270	3			
1	B	174	Total	C	N	O	S	0	0	0
			1392	896	222	271	3			
1	C	173	Total	C	N	O	S	0	0	0
			1384	892	221	268	3			
1	D	173	Total	C	N	O	S	0	0	0
			1384	892	221	268	3			

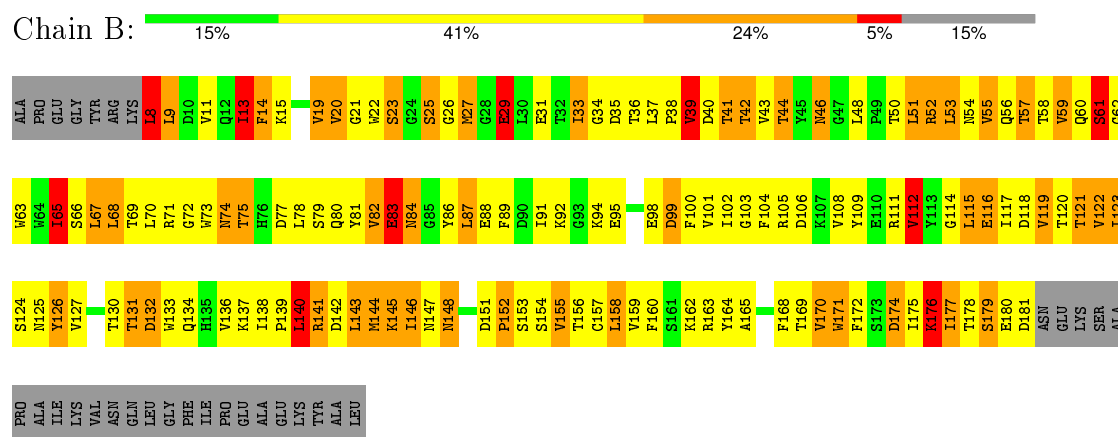
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

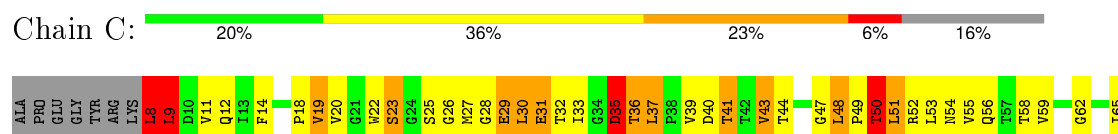
#### • Molecule 1: COG3291: FOG: PKD repeat

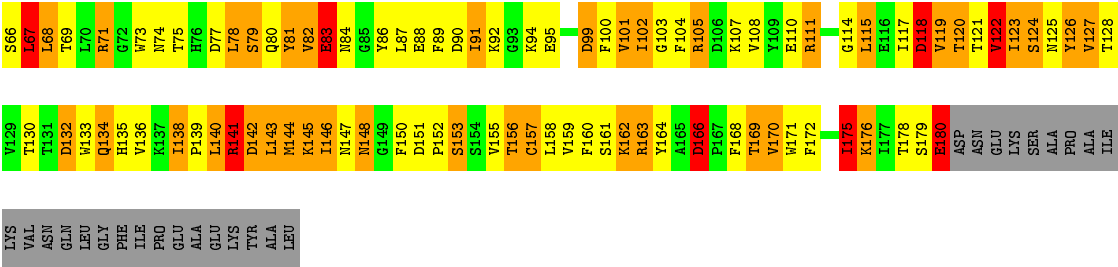


#### • Molecule 1: COG3291: FOG: PKD repeat

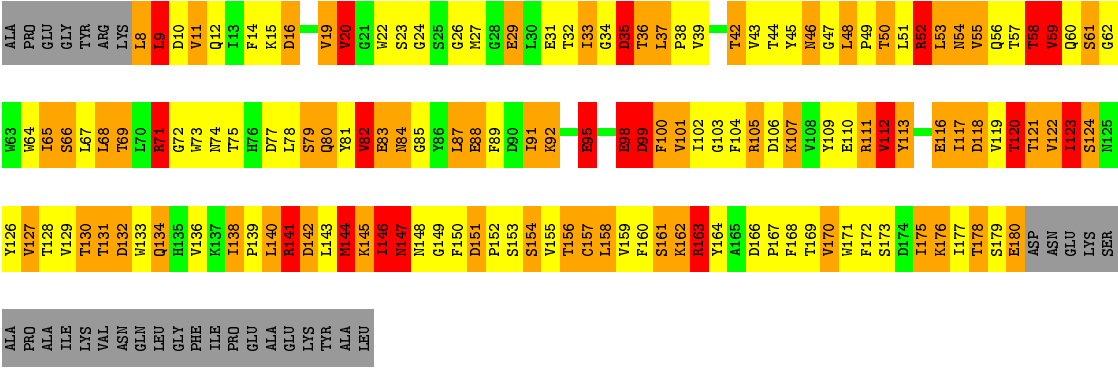
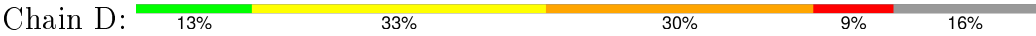


#### • Molecule 1: COG3291: FOG: PKD repeat





● Molecule 1: COG3291: FOG: PKD repeat



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.11Å 121.11Å 122.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.83 – 3.52 104.88 – 3.52	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.83-3.52) 96.1 (104.88-3.52)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.20 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.206 , 0.294 0.201 , 0.288	Depositor DCC
$R_{free}$ test set	623 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.8	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 38.7	EDS
Estimated twinning fraction	0.145 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 13225 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.79	28/1438 (1.9%)	1.58	18/1960 (0.9%)
1	B	1.72	24/1426 (1.7%)	1.55	17/1946 (0.9%)
1	C	1.67	17/1418 (1.2%)	1.53	20/1935 (1.0%)
1	D	1.73	21/1418 (1.5%)	1.53	25/1935 (1.3%)
All	All	1.73	90/5700 (1.6%)	1.54	80/7776 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
1	C	0	5
1	D	0	3
All	All	0	17

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	99	ASP	CB-CG	10.26	1.73	1.51
1	A	83	GLU	CG-CD	9.57	1.66	1.51
1	B	171	TRP	CB-CG	-8.05	1.35	1.50
1	A	100	PHE	CB-CG	-7.95	1.37	1.51
1	A	83	GLU	CB-CG	7.83	1.67	1.52
1	D	98	GLU	CG-CD	7.71	1.63	1.51
1	B	109	TYR	CE1-CZ	7.67	1.48	1.38
1	C	35	ASP	CB-CG	7.65	1.67	1.51
1	B	109	TYR	CD2-CE2	7.50	1.50	1.39
1	D	59	VAL	CA-CB	7.30	1.70	1.54
1	B	109	TYR	CE2-CZ	7.30	1.48	1.38
1	B	95	GLU	CG-CD	7.05	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	83	GLU	CG-CD	6.99	1.62	1.51
1	A	41	THR	CA-CB	6.73	1.70	1.53
1	A	145	LYS	CD-CE	6.67	1.68	1.51
1	B	109	TYR	CD1-CE1	6.66	1.49	1.39
1	B	61	SER	CA-CB	6.56	1.62	1.52
1	D	83	GLU	CB-CG	6.54	1.64	1.52
1	D	29	GLU	CG-CD	6.53	1.61	1.51
1	A	88	GLU	CG-CD	6.50	1.61	1.51
1	A	145	LYS	CB-CG	6.48	1.70	1.52
1	C	73	TRP	CB-CG	-6.38	1.38	1.50
1	B	29	GLU	CD-OE2	6.31	1.32	1.25
1	D	144	MET	CB-CG	6.31	1.71	1.51
1	C	43	VAL	CB-CG2	-6.28	1.39	1.52
1	D	180	GLU	CD-OE2	6.26	1.32	1.25
1	B	174	ASP	CB-CG	6.18	1.64	1.51
1	C	180	GLU	CB-CG	6.17	1.63	1.52
1	A	180	GLU	CG-CD	6.15	1.61	1.51
1	A	174	ASP	CB-CG	6.10	1.64	1.51
1	D	29	GLU	CD-OE1	6.09	1.32	1.25
1	A	141	ARG	CB-CG	6.08	1.69	1.52
1	A	7	LYS	CB-CG	6.05	1.68	1.52
1	B	44	THR	CA-CB	6.04	1.69	1.53
1	B	112	VAL	CB-CG2	5.98	1.65	1.52
1	D	58	THR	CA-CB	5.98	1.68	1.53
1	A	110	GLU	CG-CD	5.89	1.60	1.51
1	C	157	CYS	CB-SG	-5.89	1.72	1.81
1	D	71	ARG	CG-CD	5.86	1.66	1.51
1	C	83	GLU	CG-CD	5.85	1.60	1.51
1	B	116	GLU	CD-OE2	5.78	1.32	1.25
1	D	145	LYS	CD-CE	5.77	1.65	1.51
1	C	31	GLU	CD-OE1	5.72	1.31	1.25
1	D	180	GLU	CG-CD	5.72	1.60	1.51
1	B	163	ARG	CG-CD	5.70	1.66	1.51
1	C	142	ASP	CB-CG	5.70	1.63	1.51
1	A	137	LYS	CD-CE	5.70	1.65	1.51
1	A	81	TYR	CE1-CZ	5.68	1.46	1.38
1	D	157	CYS	CB-SG	-5.64	1.72	1.81
1	A	117	ILE	CA-CB	-5.63	1.42	1.54
1	C	81	TYR	CE1-CZ	5.61	1.45	1.38
1	A	110	GLU	CB-CG	5.61	1.62	1.52
1	C	81	TYR	CD2-CE2	5.60	1.47	1.39
1	D	98	GLU	CD-OE2	5.55	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	TYR	CZ-OH	5.55	1.47	1.37
1	D	162	LYS	CD-CE	5.53	1.65	1.51
1	A	95	GLU	CG-CD	5.52	1.60	1.51
1	B	39	VAL	CA-CB	-5.51	1.43	1.54
1	A	15	LYS	CD-CE	5.48	1.65	1.51
1	C	81	TYR	CD1-CE1	5.46	1.47	1.39
1	A	98	GLU	CG-CD	5.45	1.60	1.51
1	C	118	ASP	CB-CG	5.45	1.63	1.51
1	C	166	ASP	CB-CG	5.45	1.63	1.51
1	B	29	GLU	CD-OE1	5.44	1.31	1.25
1	C	122	VAL	CA-CB	-5.41	1.43	1.54
1	A	41	THR	CB-CG2	5.39	1.70	1.52
1	C	138	ILE	CA-CB	-5.39	1.42	1.54
1	A	83	GLU	CD-OE2	5.35	1.31	1.25
1	A	19	VAL	CA-CB	-5.35	1.43	1.54
1	B	61	SER	CB-OG	5.33	1.49	1.42
1	A	7	LYS	CG-CD	5.32	1.70	1.52
1	B	164	TYR	CD1-CE1	5.32	1.47	1.39
1	D	71	ARG	CB-CG	5.31	1.66	1.52
1	B	59	VAL	CA-CB	5.31	1.65	1.54
1	A	81	TYR	CE2-CZ	5.24	1.45	1.38
1	D	144	MET	CG-SD	5.24	1.94	1.81
1	D	162	LYS	CE-NZ	5.24	1.62	1.49
1	B	13	ILE	CA-CB	-5.23	1.42	1.54
1	D	61	SER	CA-CB	5.21	1.60	1.52
1	D	100	PHE	CE2-CZ	5.18	1.47	1.37
1	A	45	TYR	CD1-CE1	5.17	1.47	1.39
1	B	73	TRP	CB-CG	-5.14	1.41	1.50
1	B	126	TYR	CE2-CZ	5.13	1.45	1.38
1	B	155	VAL	CB-CG1	5.13	1.63	1.52
1	C	29	GLU	CG-CD	5.12	1.59	1.51
1	A	7	LYS	CD-CE	5.12	1.64	1.51
1	D	20	VAL	CB-CG2	5.09	1.63	1.52
1	A	159	VAL	CA-CB	-5.09	1.44	1.54
1	B	177	ILE	CA-CB	-5.07	1.43	1.54
1	A	55	VAL	CB-CG2	-5.06	1.42	1.52

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	LEU	CB-CG-CD1	-11.35	91.71	111.00
1	B	9	LEU	CA-CB-CG	10.44	139.31	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	LEU	CA-CB-CG	-8.90	94.84	115.30
1	B	19	VAL	CB-CA-C	-8.39	95.45	111.40
1	B	52	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	60	GLN	N-CA-CB	-7.66	96.82	110.60
1	D	112	VAL	CB-CA-C	-7.62	96.92	111.40
1	B	108	VAL	CB-CA-C	-7.53	97.09	111.40
1	D	9	LEU	CA-CB-CG	7.27	132.03	115.30
1	B	163	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	C	99	ASP	CB-CG-OD1	7.22	124.80	118.30
1	C	51	LEU	CB-CG-CD1	-7.16	98.83	111.00
1	B	163	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	D	99	ASP	CB-CG-OD1	-7.00	112.00	118.30
1	C	143	LEU	CA-CB-CG	-6.99	99.23	115.30
1	C	50	THR	CB-CA-C	-6.90	92.96	111.60
1	B	146	ILE	CB-CA-C	-6.63	98.33	111.60
1	C	67	LEU	CB-CG-CD2	-6.55	99.87	111.00
1	D	144	MET	CB-CG-SD	6.49	131.87	112.40
1	C	48	LEU	CA-CB-CG	-6.47	100.43	115.30
1	A	107	LYS	CD-CE-NZ	6.46	126.55	111.70
1	A	163	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	D	27	MET	CB-CG-SD	-6.43	93.10	112.40
1	C	30	LEU	CA-CB-CG	-6.40	100.58	115.30
1	D	48	LEU	CA-CB-CG	-6.32	100.76	115.30
1	A	178	THR	CB-CA-C	-6.31	94.56	111.60
1	B	99	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	D	162	LYS	CD-CE-NZ	6.24	126.05	111.70
1	A	19	VAL	CB-CA-C	-6.19	99.64	111.40
1	D	68	LEU	CA-CB-CG	-6.18	101.09	115.30
1	D	138	ILE	CB-CA-C	-5.96	99.67	111.60
1	D	163	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	170	VAL	CB-CA-C	-5.90	100.20	111.40
1	A	8	LEU	N-CA-C	5.89	126.91	111.00
1	A	48	LEU	CB-CG-CD1	5.87	120.97	111.00
1	B	51	LEU	CA-CB-CG	5.84	128.73	115.30
1	C	180	GLU	CB-CA-C	-5.83	98.73	110.40
1	B	176	LYS	CB-CA-C	-5.82	98.77	110.40
1	B	132	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	180	GLU	N-CA-C	5.77	126.59	111.00
1	C	35	ASP	CB-CG-OD2	5.76	123.48	118.30
1	C	144	MET	CB-CG-SD	5.70	129.50	112.40
1	D	151	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	A	67	LEU	CA-CB-CG	-5.66	102.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	VAL	CG1-CB-CG2	5.65	119.94	110.90
1	D	123	ILE	CB-CA-C	-5.65	100.30	111.60
1	A	140	LEU	CB-CG-CD2	5.64	120.59	111.00
1	D	53	LEU	CA-CB-CG	-5.58	102.46	115.30
1	D	156	THR	CB-CA-C	-5.55	96.61	111.60
1	A	118	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	D	111	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	8	LEU	N-CA-C	5.52	125.91	111.00
1	D	87	LEU	CA-CB-CG	-5.52	102.60	115.30
1	A	174	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	118	ASP	CB-CG-OD2	5.50	123.25	118.30
1	D	157	CYS	N-CA-C	5.45	125.72	111.00
1	C	9	LEU	CA-CB-CG	5.41	127.73	115.30
1	A	141	ARG	CA-CB-CG	5.39	125.26	113.40
1	D	69	THR	CB-CA-C	-5.38	97.07	111.60
1	A	137	LYS	CD-CE-NZ	5.38	124.07	111.70
1	A	111	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	120	THR	CB-CA-C	-5.30	97.29	111.60
1	D	118	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	D	120	THR	CB-CA-C	-5.28	97.35	111.60
1	D	52	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	83	GLU	N-CA-CB	-5.25	101.16	110.60
1	A	143	LEU	CA-CB-CG	5.24	127.34	115.30
1	A	141	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	11	VAL	CB-CA-C	-5.23	101.47	111.40
1	D	8	LEU	CB-CG-CD1	5.22	119.88	111.00
1	C	175	ILE	N-CA-C	-5.17	97.05	111.00
1	D	144	MET	CA-CB-CG	5.14	122.04	113.30
1	B	9	LEU	CB-CA-C	-5.11	100.49	110.20
1	D	8	LEU	N-CA-C	5.11	124.79	111.00
1	B	29	GLU	N-CA-CB	-5.07	101.47	110.60
1	D	117	ILE	CB-CA-C	-5.07	101.47	111.60
1	C	78	LEU	CB-CG-CD1	-5.06	102.39	111.00
1	B	65	ILE	CG1-CB-CG2	-5.03	100.33	111.40
1	B	33	ILE	CB-CA-C	-5.03	101.54	111.60
1	C	105	ARG	NE-CZ-NH1	-5.03	117.79	120.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	140	LEU	Peptide
1	A	145	LYS	Peptide
1	A	7	LYS	Peptide
1	B	140	LEU	Peptide
1	B	145	LYS	Peptide
1	B	179	SER	Peptide
1	B	60	GLN	Peptide
1	B	8	LEU	Peptide
1	C	120	THR	Peptide
1	C	145	LYS	Peptide
1	C	179	SER	Peptide
1	C	35	ASP	Peptide
1	C	8	LEU	Peptide
1	D	120	THR	Peptide
1	D	127	VAL	Peptide
1	D	35	ASP	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	1404	0	1377	223	0
1	B	1392	0	1355	168	0
1	C	1384	0	1351	172	0
1	D	1384	0	1351	210	0
All	All	5564	0	5434	767	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 70.

All (767) 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:D:140:LEU:HD12	1:D:144:MET:CE	1.43	1.46
1:A:89:PHE:CD1	1:A:91:ILE:HD11	1.68	1.27
1:A:89:PHE:CE1	1:A:91:ILE:HD11	1.71	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:LEU:CD1	1:D:144:MET:CE	2.24	1.15
1:D:98:GLU:OE1	1:D:168:PHE:HB3	1.48	1.13
1:C:54:ASN:HA	1:C:169:THR:HG23	1.26	1.12
1:A:50:THR:HG22	1:A:172:PHE:O	1.46	1.12
1:B:59:VAL:HG23	1:B:62:GLY:H	1.16	1.11
1:B:25:SER:HB2	1:B:29:GLU:HG3	1.33	1.10
1:A:169:THR:HG22	1:A:170:VAL:H	1.00	1.10
1:A:71:ARG:HH11	1:A:71:ARG:HG2	0.94	1.10
1:A:57:THR:HG23	1:A:58:THR:N	1.60	1.08
1:A:123:ILE:H	1:A:123:ILE:HD13	0.98	1.08
1:D:140:LEU:HD12	1:D:144:MET:HE2	1.33	1.08
1:A:169:THR:HG22	1:A:170:VAL:N	1.67	1.07
1:D:8:LEU:HD12	1:D:9:LEU:H	1.16	1.06
1:B:111:ARG:NH2	1:B:117:ILE:HD13	1.70	1.06
1:C:146:ILE:O	1:C:148:ASN:N	1.89	1.05
1:C:92:LYS:HD3	1:C:133:TRP:NE1	1.70	1.05
1:D:144:MET:HG3	1:D:150:PHE:HE2	1.17	1.05
1:B:69:THR:HA	1:B:157:CYS:HB3	1.38	1.03
1:D:10:ASP:OD2	1:D:178:THR:HG22	1.59	1.03
1:D:169:THR:HG22	1:D:170:VAL:N	1.73	1.02
1:B:100:PHE:H	1:B:123:ILE:CD1	1.72	1.02
1:D:140:LEU:CD1	1:D:144:MET:HE1	1.85	1.01
1:A:127:VAL:HG12	1:A:128:THR:O	1.59	1.01
1:C:50:THR:HG22	1:C:172:PHE:O	1.61	1.01
1:D:140:LEU:HD12	1:D:144:MET:HE1	1.03	1.01
1:C:54:ASN:CA	1:C:169:THR:HG23	1.91	1.01
1:D:48:LEU:HD13	1:D:49:PRO:HD2	1.42	0.99
1:A:16:ASP:HB3	1:A:48:LEU:HD23	1.43	0.99
1:D:50:THR:HG22	1:D:172:PHE:O	1.62	0.99
1:A:69:THR:HA	1:A:157:CYS:HB3	1.39	0.99
1:A:57:THR:HG23	1:A:58:THR:H	1.15	0.98
1:B:82:VAL:HG12	1:B:83:GLU:N	1.77	0.98
1:D:144:MET:HG3	1:D:150:PHE:CE2	1.98	0.98
1:C:20:VAL:O	1:C:69:THR:HG23	1.63	0.98
1:A:6:ARG:HG2	1:A:8:LEU:HD21	1.42	0.98
1:A:123:ILE:N	1:A:123:ILE:HD13	1.75	0.97
1:D:100:PHE:H	1:D:123:ILE:HD11	1.31	0.95
1:C:69:THR:HA	1:C:157:CYS:HB3	1.48	0.95
1:A:123:ILE:H	1:A:123:ILE:CD1	1.80	0.94
1:D:45:TYR:O	1:D:46:ASN:HB2	1.65	0.94
1:B:87:LEU:HD12	1:B:88:GLU:N	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:PHE:H	1:D:123:ILE:CD1	1.82	0.93
1:C:59:VAL:HG11	1:C:162:LYS:HD2	1.50	0.93
1:C:117:ILE:HG22	1:C:118:ASP:N	1.82	0.92
1:B:54:ASN:HB2	1:B:169:THR:HG23	1.50	0.92
1:C:67:LEU:O	1:C:68:LEU:HD23	1.70	0.92
1:A:101:VAL:CG1	1:A:120:THR:HG23	2.00	0.92
1:D:140:LEU:CD1	1:D:144:MET:HE2	1.93	0.92
1:A:88:GLU:OE1	1:A:135:HIS:CE1	2.24	0.91
1:B:77:ASP:OD1	1:B:153:SER:HB2	1.70	0.90
1:B:75:THR:HG22	1:B:154:SER:HA	1.52	0.90
1:D:82:VAL:CG1	1:D:83:GLU:N	2.36	0.89
1:D:68:LEU:O	1:D:157:CYS:HB2	1.73	0.89
1:A:169:THR:CG2	1:A:170:VAL:H	1.85	0.89
1:A:57:THR:CG2	1:A:58:THR:N	2.31	0.88
1:A:146:ILE:O	1:A:148:ASN:N	2.07	0.88
1:D:111:ARG:NH2	1:D:117:ILE:HG12	1.89	0.88
1:A:89:PHE:CE1	1:A:91:ILE:CD1	2.56	0.88
1:A:71:ARG:HG2	1:A:71:ARG:NH1	1.67	0.87
1:D:82:VAL:HG13	1:D:83:GLU:N	1.87	0.87
1:C:67:LEU:C	1:C:68:LEU:HD23	1.95	0.87
1:D:91:ILE:O	1:D:91:ILE:HD13	1.75	0.86
1:C:146:ILE:O	1:C:148:ASN:HB3	1.75	0.86
1:B:111:ARG:CZ	1:B:117:ILE:HD13	2.04	0.86
1:C:8:LEU:HG	1:C:9:LEU:N	1.86	0.86
1:C:119:VAL:HG22	1:C:150:PHE:CE1	2.11	0.86
1:B:69:THR:HA	1:B:157:CYS:CB	2.06	0.86
1:D:169:THR:CG2	1:D:170:VAL:N	2.39	0.85
1:B:121:THR:HG21	1:B:126:TYR:HE2	1.42	0.85
1:D:8:LEU:CD1	1:D:9:LEU:HD12	2.07	0.85
1:A:15:LYS:HE2	1:A:48:LEU:HD21	1.59	0.84
1:B:25:SER:CB	1:B:29:GLU:HG3	2.07	0.84
1:D:144:MET:CG	1:D:150:PHE:HE2	1.89	0.84
1:D:113:TYR:H	1:D:113:TYR:HD2	1.23	0.84
1:A:175:ILE:N	1:A:175:ILE:HD12	1.90	0.84
1:D:69:THR:HA	1:D:157:CYS:HB3	1.59	0.83
1:D:44:THR:OG1	1:D:45:TYR:N	2.06	0.83
1:D:130:THR:OG1	1:D:132:ASP:HB2	1.78	0.83
1:C:23:SER:HB3	1:C:66:SER:OG	1.76	0.83
1:C:111:ARG:NH2	1:C:117:ILE:HD12	1.93	0.83
1:B:99:ASP:OD1	1:B:123:ILE:HD13	1.79	0.82
1:A:100:PHE:H	1:A:123:ILE:HD11	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:O	1:B:145:LYS:N	2.12	0.81
1:D:100:PHE:N	1:D:123:ILE:HD11	1.95	0.81
1:B:143:LEU:N	1:B:143:LEU:HD13	1.95	0.81
1:D:20:VAL:O	1:D:69:THR:HG23	1.80	0.81
1:B:121:THR:HG21	1:B:126:TYR:CE2	2.16	0.81
1:C:54:ASN:HB2	1:C:169:THR:CG2	2.11	0.81
1:D:99:ASP:HA	1:D:123:ILE:HD11	1.62	0.81
1:A:16:ASP:CB	1:A:48:LEU:HD23	2.09	0.81
1:A:179:SER:OG	1:A:180:GLU:N	2.11	0.81
1:B:13:ILE:HG22	1:B:14:PHE:N	1.96	0.80
1:A:143:LEU:O	1:A:145:LYS:N	2.13	0.80
1:B:100:PHE:H	1:B:123:ILE:HD11	1.44	0.80
1:B:59:VAL:HG23	1:B:62:GLY:N	1.95	0.80
1:C:29:GLU:OE2	1:C:29:GLU:N	2.14	0.80
1:C:146:ILE:C	1:C:148:ASN:H	1.84	0.80
1:B:143:LEU:CD1	1:B:143:LEU:N	2.44	0.79
1:C:43:VAL:O	1:C:43:VAL:HG12	1.81	0.79
1:B:136:VAL:HG22	1:B:137:LYS:N	1.97	0.79
1:C:9:LEU:O	1:C:81:TYR:OH	1.99	0.79
1:C:54:ASN:CB	1:C:169:THR:HG23	2.12	0.79
1:C:111:ARG:HG3	1:C:114:GLY:O	1.83	0.79
1:C:102:ILE:HD12	1:C:160:PHE:HE2	1.48	0.79
1:A:100:PHE:O	1:A:123:ILE:CD1	2.31	0.79
1:C:68:LEU:O	1:C:157:CYS:HB2	1.83	0.79
1:C:55:VAL:HG13	1:C:168:PHE:H	1.48	0.79
1:D:59:VAL:HG23	1:D:62:GLY:H	1.48	0.78
1:C:111:ARG:HH21	1:C:117:ILE:HD12	1.49	0.78
1:D:22:TRP:CH2	1:D:24:GLY:HA3	2.18	0.78
1:B:146:ILE:O	1:B:148:ASN:N	2.14	0.77
1:B:68:LEU:O	1:B:157:CYS:HB2	1.84	0.77
1:B:111:ARG:NH2	1:B:117:ILE:CD1	2.46	0.77
1:D:163:ARG:HD3	1:D:164:TYR:CE2	2.20	0.77
1:D:105:ARG:HA	1:D:117:ILE:O	1.83	0.77
1:B:25:SER:HB2	1:B:29:GLU:CG	2.14	0.77
1:D:8:LEU:HD12	1:D:9:LEU:N	1.99	0.77
1:A:22:TRP:O	1:A:67:LEU:HB2	1.85	0.76
1:C:111:ARG:CG	1:C:114:GLY:O	2.33	0.76
1:C:68:LEU:N	1:C:68:LEU:HD23	1.98	0.76
1:B:125:ASN:O	1:D:20:VAL:HG11	1.84	0.76
1:B:82:VAL:CG1	1:B:83:GLU:N	2.48	0.76
1:B:169:THR:HG22	1:B:170:VAL:N	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:VAL:HG11	1:C:134:GLN:NE2	2.00	0.76
1:B:136:VAL:CG2	1:B:137:LYS:N	2.48	0.76
1:A:119:VAL:HG21	1:A:143:LEU:HB3	1.68	0.76
1:D:8:LEU:HD12	1:D:9:LEU:HD12	1.66	0.75
1:A:101:VAL:HG11	1:A:120:THR:HG23	1.67	0.75
1:D:91:ILE:C	1:D:91:ILE:HD13	2.07	0.75
1:C:92:LYS:HD3	1:C:133:TRP:CE2	2.21	0.75
1:C:117:ILE:HG22	1:C:118:ASP:H	1.48	0.75
1:D:12:GLN:NE2	1:D:175:ILE:O	2.19	0.74
1:D:55:VAL:HG13	1:D:168:PHE:H	1.52	0.74
1:D:179:SER:O	1:D:180:GLU:HG3	1.87	0.74
1:D:91:ILE:HA	1:D:133:TRP:CZ3	2.23	0.74
1:A:16:ASP:HB3	1:A:48:LEU:CD2	2.17	0.74
1:A:55:VAL:HG23	1:A:168:PHE:H	1.52	0.74
1:D:139:PRO:O	1:D:142:ASP:OD1	2.06	0.74
1:C:117:ILE:CG2	1:C:118:ASP:N	2.50	0.73
1:C:143:LEU:H	1:C:143:LEU:HD12	1.51	0.73
1:D:123:ILE:HG12	1:D:124:SER:H	1.53	0.73
1:B:140:LEU:O	1:B:141:ARG:C	2.25	0.73
1:C:87:LEU:HD12	1:C:104:PHE:HZ	1.53	0.73
1:C:130:THR:C	1:C:132:ASP:H	1.92	0.73
1:A:54:ASN:HD22	1:A:55:VAL:N	1.86	0.73
1:D:95:GLU:O	1:D:95:GLU:HG2	1.89	0.73
1:B:140:LEU:HD12	1:B:144:MET:HG3	1.71	0.72
1:C:127:VAL:CG1	1:C:134:GLN:NE2	2.52	0.72
1:A:130:THR:C	1:A:132:ASP:H	1.93	0.72
1:A:143:LEU:C	1:A:145:LYS:H	1.87	0.72
1:C:54:ASN:HA	1:C:169:THR:CG2	2.13	0.72
1:D:169:THR:HG21	1:D:171:TRP:CH2	2.24	0.72
1:A:71:ARG:CG	1:A:71:ARG:NH1	2.51	0.72
1:B:170:VAL:HG13	1:B:171:TRP:N	2.04	0.72
1:A:54:ASN:ND2	1:A:168:PHE:O	2.23	0.72
1:A:159:VAL:O	1:A:160:PHE:HD1	1.72	0.72
1:B:121:THR:HG23	1:B:122:VAL:N	2.04	0.72
1:A:175:ILE:N	1:A:175:ILE:CD1	2.53	0.71
1:A:100:PHE:CD2	1:A:100:PHE:N	2.52	0.71
1:C:23:SER:HB3	1:C:66:SER:CB	2.19	0.71
1:A:15:LYS:HE2	1:A:48:LEU:CD2	2.20	0.71
1:D:131:THR:O	1:D:131:THR:HG22	1.91	0.71
1:C:54:ASN:HB2	1:C:169:THR:HG21	1.73	0.71
1:B:174:ASP:OD1	1:B:176:LYS:HE2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PHE:HB3	1:A:175:ILE:HA	1.71	0.71
1:C:92:LYS:CD	1:C:133:TRP:NE1	2.50	0.71
1:D:146:ILE:O	1:D:148:ASN:N	2.22	0.70
1:A:54:ASN:ND2	1:A:55:VAL:N	2.39	0.70
1:B:143:LEU:C	1:B:145:LYS:H	1.92	0.70
1:A:89:PHE:CB	1:A:175:ILE:HG13	2.21	0.70
1:C:117:ILE:CG2	1:C:118:ASP:H	2.05	0.70
1:D:69:THR:HA	1:D:157:CYS:CB	2.21	0.70
1:A:89:PHE:CD1	1:A:91:ILE:CD1	2.62	0.70
1:A:101:VAL:HG12	1:A:102:ILE:N	2.05	0.70
1:B:125:ASN:N	1:B:125:ASN:HD22	1.89	0.70
1:C:140:LEU:O	1:C:141:ARG:C	2.28	0.69
1:A:14:PHE:C	1:A:14:PHE:CD1	2.65	0.69
1:A:22:TRP:CH2	1:A:24:GLY:HA3	2.27	0.69
1:A:89:PHE:HE1	1:A:91:ILE:HD11	1.51	0.69
1:C:40:ASP:OD2	1:C:41:THR:N	2.25	0.69
1:C:30:LEU:HD12	1:C:31:GLU:N	2.07	0.69
1:D:91:ILE:HG12	1:D:170:VAL:HG23	1.73	0.69
1:B:88:GLU:HB3	1:B:137:LYS:HG2	1.74	0.69
1:B:54:ASN:HD22	1:B:55:VAL:N	1.91	0.69
1:D:82:VAL:CG1	1:D:83:GLU:H	2.06	0.69
1:C:121:THR:OG1	1:C:122:VAL:N	2.25	0.69
1:C:54:ASN:CB	1:C:169:THR:CG2	2.69	0.69
1:A:82:VAL:HG12	1:A:83:GLU:N	2.06	0.69
1:A:22:TRP:CZ3	1:A:24:GLY:N	2.61	0.69
1:B:143:LEU:H	1:B:143:LEU:HD13	1.55	0.68
1:B:105:ARG:HA	1:B:117:ILE:O	1.92	0.68
1:D:22:TRP:CE3	1:D:23:SER:N	2.61	0.68
1:A:101:VAL:HG13	1:A:120:THR:HG23	1.74	0.68
1:C:111:ARG:CZ	1:C:117:ILE:HD12	2.23	0.68
1:B:106:ASP:O	1:B:116:GLU:HB3	1.94	0.68
1:B:100:PHE:N	1:B:123:ILE:HD11	2.09	0.68
1:B:100:PHE:N	1:B:123:ILE:CD1	2.53	0.68
1:C:79:SER:O	1:C:82:VAL:HG23	1.93	0.68
1:B:136:VAL:CG2	1:B:137:LYS:H	2.07	0.67
1:C:102:ILE:HG13	1:C:103:GLY:N	2.07	0.67
1:A:119:VAL:CG2	1:A:143:LEU:HB3	2.24	0.67
1:A:140:LEU:HD12	1:A:144:MET:CE	2.24	0.67
1:C:141:ARG:O	1:C:145:LYS:HG3	1.94	0.67
1:D:159:VAL:HG12	1:D:160:PHE:N	2.10	0.67
1:C:108:VAL:O	1:C:115:LEU:HD13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASP:C	1:A:91:ILE:HD12	2.15	0.67
1:D:170:VAL:HG22	1:D:171:TRP:N	2.10	0.67
1:A:19:VAL:HG23	1:A:19:VAL:O	1.94	0.66
1:A:37:LEU:HB2	1:A:51:LEU:HD11	1.76	0.66
1:B:87:LEU:HD11	1:B:89:PHE:HD2	1.59	0.66
1:B:130:THR:C	1:B:132:ASP:H	1.98	0.66
1:A:86:TYR:N	1:A:140:LEU:HD23	2.11	0.66
1:B:140:LEU:O	1:B:142:ASP:N	2.29	0.66
1:C:69:THR:HA	1:C:157:CYS:CB	2.23	0.66
1:B:170:VAL:CG1	1:B:171:TRP:N	2.57	0.66
1:D:91:ILE:HG12	1:D:170:VAL:CG2	2.26	0.66
1:C:30:LEU:HD12	1:C:31:GLU:H	1.59	0.66
1:D:113:TYR:HD2	1:D:113:TYR:N	1.91	0.66
1:C:8:LEU:HD12	1:C:9:LEU:HD23	1.77	0.66
1:B:14:PHE:C	1:B:14:PHE:CD2	2.66	0.66
1:A:89:PHE:HD1	1:A:91:ILE:HD11	1.46	0.65
1:A:86:TYR:CE2	1:A:137:LYS:HD3	2.30	0.65
1:D:53:LEU:HB3	1:D:170:VAL:HG13	1.77	0.65
1:A:37:LEU:HD13	1:A:37:LEU:N	2.11	0.65
1:A:40:ASP:HB2	1:A:52:ARG:NH1	2.11	0.65
1:C:101:VAL:HG23	1:C:161:SER:O	1.96	0.65
1:B:50:THR:HB	1:B:172:PHE:O	1.97	0.65
1:A:140:LEU:HD21	1:A:177:ILE:CG2	2.26	0.65
1:C:55:VAL:HG22	1:C:55:VAL:O	1.95	0.65
1:D:59:VAL:HG23	1:D:62:GLY:N	2.11	0.65
1:D:170:VAL:CG2	1:D:171:TRP:N	2.59	0.64
1:B:99:ASP:OD1	1:B:123:ILE:CD1	2.45	0.64
1:D:158:LEU:HD22	1:D:159:VAL:N	2.12	0.64
1:C:31:GLU:OE1	1:C:52:ARG:NH1	2.30	0.64
1:A:100:PHE:O	1:A:123:ILE:HD13	1.98	0.64
1:B:53:LEU:HD23	1:B:172:PHE:HE1	1.62	0.64
1:C:67:LEU:HD21	1:C:105:ARG:NH1	2.11	0.64
1:D:10:ASP:OD2	1:D:178:THR:CG2	2.40	0.64
1:D:158:LEU:HD22	1:D:159:VAL:H	1.61	0.64
1:C:101:VAL:HG13	1:C:122:VAL:HG13	1.80	0.64
1:B:87:LEU:HD11	1:B:89:PHE:CD2	2.33	0.64
1:A:100:PHE:HA	1:A:163:ARG:HB3	1.79	0.64
1:D:99:ASP:OD1	1:D:124:SER:OG	2.15	0.64
1:B:102:ILE:HA	1:B:159:VAL:O	1.97	0.64
1:C:48:LEU:HD23	1:C:48:LEU:N	2.12	0.64
1:C:78:LEU:O	1:C:80:GLN:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HD12	1:A:52:ARG:N	2.14	0.63
1:C:87:LEU:HD12	1:C:104:PHE:CZ	2.34	0.63
1:D:106:ASP:HB2	1:D:154:SER:O	1.99	0.63
1:C:22:TRP:O	1:C:67:LEU:HD12	1.98	0.63
1:D:179:SER:OG	1:D:180:GLU:N	2.30	0.63
1:B:20:VAL:O	1:B:69:THR:HG23	1.99	0.63
1:D:130:THR:C	1:D:132:ASP:H	2.02	0.63
1:C:126:TYR:CD2	1:C:126:TYR:N	2.63	0.63
1:C:111:ARG:NE	1:C:117:ILE:HD12	2.13	0.63
1:B:8:LEU:HG	1:B:9:LEU:N	2.12	0.63
1:D:48:LEU:N	1:D:48:LEU:HD22	2.14	0.62
1:A:54:ASN:HD22	1:A:55:VAL:H	1.45	0.62
1:A:6:ARG:CG	1:A:8:LEU:HD21	2.25	0.62
1:A:64:TRP:CD1	1:A:162:LYS:HB2	2.35	0.62
1:D:99:ASP:CA	1:D:123:ILE:HD11	2.30	0.62
1:C:172:PHE:HB3	1:C:175:ILE:HD11	1.81	0.62
1:B:82:VAL:HG12	1:B:83:GLU:H	1.61	0.62
1:B:54:ASN:ND2	1:B:55:VAL:N	2.47	0.62
1:D:123:ILE:HG12	1:D:124:SER:N	2.15	0.61
1:C:20:VAL:O	1:C:69:THR:CG2	2.45	0.61
1:B:13:ILE:HG22	1:B:175:ILE:HB	1.81	0.61
1:A:26:GLY:HA3	1:A:61:SER:OG	2.00	0.61
1:D:54:ASN:HD22	1:D:55:VAL:N	1.98	0.61
1:C:54:ASN:CA	1:C:169:THR:CG2	2.74	0.61
1:B:100:PHE:H	1:B:123:ILE:HD13	1.61	0.61
1:D:91:ILE:HD11	1:D:129:VAL:HG13	1.80	0.61
1:C:103:GLY:O	1:C:158:LEU:HD12	2.00	0.61
1:D:87:LEU:HG	1:D:88:GLU:N	2.16	0.61
1:C:59:VAL:CG1	1:C:162:LYS:HD2	2.28	0.61
1:B:57:THR:HG22	1:B:58:THR:H	1.66	0.61
1:C:65:ILE:HG13	1:C:66:SER:N	2.14	0.61
1:C:88:GLU:OE2	1:C:135:HIS:CE1	2.53	0.61
1:D:55:VAL:O	1:D:55:VAL:HG22	2.00	0.60
1:C:111:ARG:HE	1:C:117:ILE:CD1	2.14	0.60
1:A:151:ASP:C	1:A:153:SER:H	2.05	0.60
1:B:125:ASN:N	1:B:125:ASN:ND2	2.49	0.60
1:B:104:PHE:HE1	1:B:158:LEU:HB2	1.67	0.60
1:A:57:THR:OG1	1:B:34:GLY:N	2.35	0.60
1:D:16:ASP:HB3	1:D:48:LEU:HD12	1.83	0.60
1:A:33:ILE:CG2	1:A:33:ILE:O	2.48	0.60
1:C:59:VAL:HG11	1:C:162:LYS:CD	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:LYS:O	1:D:170:VAL:HG23	2.01	0.60
1:C:108:VAL:CG1	1:C:111:ARG:HB3	2.31	0.60
1:C:101:VAL:CG1	1:C:122:VAL:HG13	2.31	0.60
1:C:130:THR:C	1:C:132:ASP:N	2.54	0.60
1:A:151:ASP:O	1:A:153:SER:N	2.35	0.60
1:B:179:SER:OG	1:B:180:GLU:N	2.35	0.60
1:B:139:PRO:HG2	1:B:142:ASP:OD2	2.01	0.59
1:B:65:ILE:HD12	1:B:66:SER:N	2.18	0.59
1:C:119:VAL:HG22	1:C:150:PHE:CD1	2.37	0.59
1:B:133:TRP:CE3	1:B:133:TRP:HA	2.36	0.59
1:A:123:ILE:O	1:A:124:SER:C	2.40	0.59
1:D:82:VAL:HG12	1:D:83:GLU:H	1.67	0.59
1:B:8:LEU:HG	1:B:9:LEU:H	1.65	0.59
1:A:78:LEU:O	1:A:80:GLN:N	2.34	0.59
1:B:33:ILE:O	1:B:34:GLY:C	2.40	0.59
1:C:92:LYS:HD3	1:C:133:TRP:HE1	1.63	0.59
1:D:148:ASN:OD1	1:D:149:GLY:N	2.36	0.59
1:C:102:ILE:HD12	1:C:160:PHE:CE2	2.34	0.59
1:D:53:LEU:HG	1:D:53:LEU:O	2.03	0.59
1:D:51:LEU:HB3	1:D:172:PHE:HB2	1.84	0.59
1:A:127:VAL:CG1	1:A:128:THR:O	2.44	0.59
1:C:108:VAL:HG12	1:C:111:ARG:HB3	1.84	0.59
1:B:87:LEU:HD12	1:B:87:LEU:C	2.22	0.59
1:D:87:LEU:H	1:D:140:LEU:CD2	2.15	0.59
1:D:104:PHE:N	1:D:104:PHE:CD2	2.71	0.59
1:D:95:GLU:CG	1:D:95:GLU:O	2.51	0.59
1:C:164:TYR:HB3	1:C:166:ASP:OD2	2.03	0.59
1:B:169:THR:HG22	1:B:170:VAL:H	1.66	0.58
1:D:148:ASN:OD1	1:D:148:ASN:C	2.39	0.58
1:C:8:LEU:HG	1:C:9:LEU:H	1.67	0.58
1:D:89:PHE:CD2	1:D:89:PHE:N	2.70	0.58
1:A:88:GLU:OE1	1:A:135:HIS:HE1	1.78	0.58
1:A:13:ILE:HG12	1:A:70:LEU:CD2	2.33	0.58
1:B:104:PHE:CE1	1:B:158:LEU:HB2	2.37	0.58
1:D:126:TYR:CD1	1:D:138:ILE:HG13	2.38	0.58
1:A:71:ARG:O	1:A:72:GLY:C	2.39	0.58
1:C:8:LEU:CG	1:C:9:LEU:N	2.62	0.58
1:C:110:GLU:N	1:C:110:GLU:OE1	2.33	0.58
1:D:87:LEU:HD12	1:D:176:LYS:O	2.04	0.58
1:C:141:ARG:O	1:C:145:LYS:CG	2.52	0.58
1:D:169:THR:CG2	1:D:170:VAL:H	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ILE:HG22	1:D:139:PRO:O	2.04	0.58
1:C:78:LEU:HG	1:C:155:VAL:HG21	1.85	0.58
1:C:176:LYS:HG3	1:C:178:THR:HG23	1.85	0.58
1:D:48:LEU:N	1:D:48:LEU:CD2	2.67	0.58
1:A:130:THR:C	1:A:132:ASP:N	2.57	0.58
1:A:59:VAL:HG12	1:A:62:GLY:H	1.69	0.58
1:B:103:GLY:HA3	1:B:119:VAL:O	2.04	0.57
1:B:39:VAL:HG22	1:B:39:VAL:O	2.02	0.57
1:D:140:LEU:O	1:D:141:ARG:C	2.41	0.57
1:A:127:VAL:HG21	1:A:136:VAL:HG11	1.85	0.57
1:C:87:LEU:H	1:C:140:LEU:CD2	2.17	0.57
1:B:53:LEU:HD23	1:B:172:PHE:CE1	2.38	0.57
1:D:91:ILE:HA	1:D:133:TRP:HZ3	1.68	0.57
1:B:41:THR:C	1:B:43:VAL:H	2.07	0.57
1:B:71:ARG:O	1:B:72:GLY:C	2.42	0.57
1:D:53:LEU:C	1:D:53:LEU:HD12	2.24	0.57
1:D:22:TRP:CZ3	1:D:24:GLY:HA3	2.39	0.57
1:A:68:LEU:O	1:A:157:CYS:HB2	2.05	0.57
1:D:36:THR:HG23	1:D:37:LEU:N	2.20	0.57
1:D:45:TYR:O	1:D:46:ASN:CB	2.47	0.57
1:D:11:VAL:HG23	1:D:177:ILE:HB	1.86	0.57
1:A:88:GLU:C	1:A:89:PHE:CD2	2.79	0.57
1:A:50:THR:CG2	1:A:172:PHE:O	2.38	0.57
1:D:102:ILE:HG22	1:D:121:THR:O	2.05	0.57
1:B:130:THR:C	1:B:132:ASP:N	2.58	0.57
1:B:91:ILE:HA	1:B:133:TRP:HZ3	1.68	0.57
1:D:170:VAL:CG2	1:D:171:TRP:H	2.18	0.56
1:D:100:PHE:H	1:D:123:ILE:HD13	1.67	0.56
1:D:169:THR:HG21	1:D:171:TRP:CZ2	2.40	0.56
1:A:22:TRP:CE3	1:A:23:SER:N	2.73	0.56
1:C:8:LEU:CD1	1:C:9:LEU:H	2.18	0.56
1:D:89:PHE:HB3	1:D:175:ILE:HA	1.87	0.56
1:B:156:THR:HG23	1:B:157:CYS:SG	2.45	0.56
1:B:99:ASP:HA	1:B:123:ILE:HD11	1.87	0.56
1:B:123:ILE:H	1:B:123:ILE:HD13	1.70	0.56
1:C:67:LEU:H	1:C:67:LEU:HD12	1.71	0.56
1:D:156:THR:OG1	1:D:157:CYS:N	2.38	0.56
1:D:12:GLN:NE2	1:D:14:PHE:O	2.39	0.56
1:D:151:ASP:O	1:D:154:SER:HB2	2.06	0.56
1:A:89:PHE:HE1	1:A:91:ILE:CD1	2.14	0.56
1:A:14:PHE:CD2	1:A:51:LEU:HD23	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LYS:HG2	1:A:48:LEU:HD22	1.86	0.56
1:A:56:GLN:HB3	1:B:33:ILE:HD12	1.87	0.56
1:A:33:ILE:HG22	1:A:33:ILE:O	2.05	0.56
1:A:23:SER:CB	1:A:37:LEU:CD1	2.83	0.56
1:C:86:TYR:HA	1:C:138:ILE:O	2.06	0.56
1:A:104:PHE:HB2	1:A:119:VAL:HG12	1.88	0.56
1:C:51:LEU:HB3	1:C:172:PHE:HB2	1.88	0.56
1:B:124:SER:OG	1:B:125:ASN:ND2	2.39	0.56
1:A:72:GLY:O	1:A:73:TRP:HB2	2.07	0.55
1:D:121:THR:HG23	1:D:122:VAL:N	2.21	0.55
1:C:8:LEU:HB3	1:C:180:GLU:HG2	1.87	0.55
1:D:106:ASP:O	1:D:116:GLU:HB3	2.07	0.55
1:A:22:TRP:CZ3	1:A:24:GLY:CA	2.89	0.55
1:D:131:THR:CG2	1:D:131:THR:O	2.54	0.55
1:B:156:THR:CG2	1:B:157:CYS:N	2.68	0.55
1:D:113:TYR:CD2	1:D:113:TYR:N	2.62	0.55
1:A:98:GLU:H	1:A:129:VAL:HG21	1.71	0.55
1:A:151:ASP:O	1:A:154:SER:N	2.38	0.55
1:A:87:LEU:HD12	1:A:88:GLU:N	2.22	0.55
1:C:8:LEU:HD12	1:C:9:LEU:H	1.72	0.55
1:A:148:ASN:OD1	1:A:148:ASN:C	2.45	0.55
1:C:54:ASN:HD22	1:C:169:THR:CG2	2.20	0.55
1:C:143:LEU:C	1:C:145:LYS:H	2.09	0.55
1:B:8:LEU:HD23	1:B:8:LEU:O	2.07	0.55
1:D:59:VAL:HG23	1:D:62:GLY:CA	2.37	0.55
1:A:127:VAL:CG2	1:A:136:VAL:HG11	2.36	0.55
1:A:140:LEU:CD1	1:A:144:MET:CE	2.85	0.55
1:A:101:VAL:HG11	1:A:120:THR:CG2	2.36	0.55
1:A:133:TRP:CE3	1:A:133:TRP:HA	2.41	0.55
1:B:117:ILE:CG2	1:B:118:ASP:N	2.68	0.55
1:B:57:THR:CG2	1:B:58:THR:H	2.19	0.55
1:A:102:ILE:HG22	1:A:121:THR:HG23	1.90	0.54
1:A:23:SER:OG	1:A:37:LEU:HD11	2.07	0.54
1:A:67:LEU:C	1:A:68:LEU:HD13	2.28	0.54
1:C:111:ARG:HE	1:C:117:ILE:HD12	1.72	0.54
1:C:23:SER:HA	1:C:65:ILE:O	2.07	0.54
1:C:88:GLU:OE2	1:C:135:HIS:HE1	1.89	0.54
1:D:72:GLY:O	1:D:73:TRP:HB2	2.06	0.54
1:B:102:ILE:HG21	1:B:123:ILE:HG22	1.89	0.54
1:D:117:ILE:HG22	1:D:118:ASP:N	2.23	0.54
1:A:78:LEU:O	1:A:81:TYR:HD1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LEU:HG	1:B:159:VAL:N	2.21	0.54
1:C:151:ASP:C	1:C:151:ASP:OD1	2.46	0.54
1:D:92:LYS:HB3	1:D:133:TRP:CD2	2.42	0.54
1:B:125:ASN:C	1:D:20:VAL:HG11	2.27	0.54
1:D:78:LEU:O	1:D:80:GLN:N	2.40	0.54
1:A:140:LEU:CD1	1:A:144:MET:HE3	2.38	0.54
1:A:174:ASP:C	1:A:175:ILE:HD12	2.27	0.54
1:C:37:LEU:HD23	1:C:68:LEU:HD11	1.89	0.54
1:C:8:LEU:CG	1:C:9:LEU:H	2.21	0.54
1:B:31:GLU:CD	1:B:52:ARG:HH11	2.10	0.54
1:A:89:PHE:HB3	1:A:175:ILE:HG13	1.89	0.54
1:C:19:VAL:O	1:C:36:THR:HG21	2.07	0.54
1:A:101:VAL:HG12	1:A:102:ILE:H	1.73	0.54
1:B:22:TRP:HB3	1:B:67:LEU:HD12	1.90	0.53
1:B:20:VAL:HG23	1:B:69:THR:OG1	2.09	0.53
1:D:112:VAL:HG23	1:D:113:TYR:N	2.24	0.53
1:C:122:VAL:HG11	1:C:163:ARG:HD3	1.90	0.53
1:A:159:VAL:C	1:A:160:PHE:CD1	2.82	0.53
1:A:22:TRP:CZ3	1:A:24:GLY:HA3	2.44	0.53
1:A:101:VAL:CG1	1:A:102:ILE:N	2.71	0.53
1:D:103:GLY:O	1:D:159:VAL:N	2.41	0.53
1:A:117:ILE:HG22	1:A:118:ASP:H	1.73	0.53
1:B:136:VAL:HG23	1:B:137:LYS:H	1.73	0.53
1:D:33:ILE:O	1:D:34:GLY:C	2.47	0.53
1:A:127:VAL:HG12	1:A:128:THR:N	2.24	0.53
1:D:66:SER:HB3	1:D:160:PHE:HB2	1.90	0.53
1:D:65:ILE:HG13	1:D:66:SER:N	2.22	0.53
1:B:8:LEU:CD2	1:B:179:SER:HB3	2.39	0.53
1:B:66:SER:O	1:B:159:VAL:HA	2.08	0.53
1:C:105:ARG:HA	1:C:117:ILE:O	2.08	0.53
1:A:117:ILE:HG22	1:A:118:ASP:N	2.23	0.53
1:A:50:THR:HG21	1:A:171:TRP:HB3	1.91	0.53
1:C:101:VAL:HG13	1:C:122:VAL:CG1	2.38	0.53
1:B:71:ARG:O	1:B:74:ASN:HB2	2.08	0.53
1:A:70:LEU:HG	1:A:157:CYS:HA	1.91	0.53
1:B:31:GLU:OE1	1:B:52:ARG:NH1	2.33	0.53
1:D:88:GLU:C	1:D:89:PHE:HD2	2.12	0.53
1:A:48:LEU:HB3	1:A:49:PRO:HD2	1.90	0.53
1:D:106:ASP:C	1:D:106:ASP:OD1	2.47	0.52
1:A:19:VAL:HG23	1:A:36:THR:OG1	2.08	0.52
1:C:140:LEU:O	1:C:142:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:O	1:A:81:TYR:N	2.36	0.52
1:C:89:PHE:HE1	1:C:91:ILE:HG21	1.74	0.52
1:D:143:LEU:C	1:D:145:LYS:H	2.13	0.52
1:A:159:VAL:O	1:A:160:PHE:CD1	2.60	0.52
1:A:13:ILE:HG12	1:A:70:LEU:HD22	1.91	0.52
1:D:67:LEU:HD23	1:D:159:VAL:HG22	1.91	0.52
1:D:111:ARG:CG	1:D:113:TYR:HE2	2.22	0.52
1:D:87:LEU:N	1:D:140:LEU:CD2	2.72	0.52
1:D:8:LEU:CD1	1:D:9:LEU:H	2.05	0.52
1:B:117:ILE:HG22	1:B:118:ASP:N	2.24	0.52
1:D:163:ARG:HD3	1:D:164:TYR:CZ	2.45	0.52
1:A:45:TYR:O	1:A:46:ASN:OD1	2.27	0.52
1:A:142:ASP:N	1:A:142:ASP:OD2	2.41	0.52
1:D:43:VAL:O	1:D:43:VAL:HG12	2.09	0.52
1:D:130:THR:C	1:D:132:ASP:N	2.63	0.52
1:D:109:TYR:N	1:D:110:GLU:OE1	2.42	0.52
1:A:131:THR:O	1:A:131:THR:HG22	2.10	0.52
1:C:153:SER:O	1:C:153:SER:OG	2.24	0.51
1:B:143:LEU:C	1:B:145:LYS:N	2.61	0.51
1:D:29:GLU:HG2	1:D:59:VAL:HG12	1.93	0.51
1:D:64:TRP:CZ2	1:D:162:LYS:HA	2.45	0.51
1:C:124:SER:HA	1:C:127:VAL:O	2.10	0.51
1:D:126:TYR:CD2	1:D:126:TYR:N	2.78	0.51
1:A:13:ILE:HG21	1:A:158:LEU:HD22	1.93	0.51
1:A:93:GLY:HA2	1:A:170:VAL:HA	1.92	0.51
1:C:146:ILE:O	1:C:148:ASN:CB	2.51	0.51
1:A:146:ILE:C	1:A:148:ASN:H	2.09	0.51
1:D:130:THR:OG1	1:D:132:ASP:CB	2.56	0.51
1:D:78:LEU:HD12	1:D:155:VAL:HG21	1.91	0.51
1:D:38:PRO:HG2	1:D:52:ARG:HB3	1.93	0.51
1:D:159:VAL:CG1	1:D:160:PHE:N	2.74	0.51
1:A:126:TYR:O	1:A:127:VAL:HG22	2.10	0.51
1:D:150:PHE:O	1:D:152:PRO:HD3	2.11	0.51
1:A:140:LEU:HD12	1:A:144:MET:HE3	1.93	0.51
1:A:162:LYS:HG2	1:A:163:ARG:N	2.25	0.51
1:D:143:LEU:O	1:D:145:LYS:N	2.44	0.51
1:D:101:VAL:HG23	1:D:161:SER:O	2.10	0.51
1:B:54:ASN:HD22	1:B:55:VAL:H	1.59	0.50
1:A:86:TYR:HA	1:A:138:ILE:O	2.11	0.50
1:A:104:PHE:HB2	1:A:119:VAL:CG1	2.42	0.50
1:A:97:GLY:HA2	1:A:129:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:THR:OG1	1:A:157:CYS:N	2.44	0.50
1:B:77:ASP:OD1	1:B:153:SER:CB	2.51	0.50
1:C:28:GLY:N	1:C:29:GLU:OE2	2.44	0.50
1:C:127:VAL:HG12	1:C:134:GLN:NE2	2.24	0.50
1:C:30:LEU:CD1	1:C:54:ASN:O	2.60	0.50
1:B:114:GLY:HA3	1:B:117:ILE:HD11	1.93	0.50
1:D:151:ASP:C	1:D:153:SER:H	2.15	0.50
1:D:151:ASP:O	1:D:153:SER:N	2.45	0.50
1:A:139:PRO:HB2	1:A:142:ASP:OD2	2.10	0.50
1:A:159:VAL:C	1:A:160:PHE:HD1	2.15	0.50
1:D:75:THR:HA	1:D:155:VAL:O	2.11	0.50
1:D:140:LEU:HD13	1:D:144:MET:CE	2.35	0.50
1:D:130:THR:HG22	1:D:134:GLN:OE1	2.12	0.50
1:B:91:ILE:CA	1:B:133:TRP:HZ3	2.24	0.50
1:A:158:LEU:C	1:A:159:VAL:HG23	2.32	0.50
1:B:8:LEU:C	1:B:8:LEU:HD23	2.32	0.50
1:A:23:SER:CB	1:A:37:LEU:HD11	2.42	0.49
1:B:119:VAL:CG2	1:B:143:LEU:HB3	2.42	0.49
1:D:22:TRP:CZ3	1:D:24:GLY:CA	2.95	0.49
1:A:151:ASP:C	1:A:151:ASP:OD1	2.50	0.49
1:D:98:GLU:OE2	1:D:98:GLU:HA	2.11	0.49
1:A:48:LEU:CB	1:A:49:PRO:HD2	2.42	0.49
1:D:66:SER:CB	1:D:160:PHE:HB2	2.42	0.49
1:B:13:ILE:HG22	1:B:14:PHE:H	1.76	0.49
1:B:31:GLU:CD	1:B:52:ARG:NH1	2.66	0.49
1:D:123:ILE:CG1	1:D:124:SER:N	2.76	0.49
1:A:97:GLY:CA	1:A:129:VAL:HG23	2.42	0.49
1:A:140:LEU:O	1:A:141:ARG:C	2.51	0.49
1:C:19:VAL:HG13	1:C:20:VAL:N	2.27	0.49
1:A:6:ARG:HB3	1:A:8:LEU:CD2	2.43	0.49
1:C:47:GLY:C	1:C:48:LEU:HD23	2.32	0.49
1:A:15:LYS:CE	1:A:48:LEU:HD21	2.39	0.49
1:B:29:GLU:OE1	1:B:59:VAL:HB	2.13	0.49
1:D:67:LEU:HB3	1:D:157:CYS:SG	2.52	0.49
1:D:31:GLU:O	1:D:38:PRO:HD3	2.12	0.49
1:B:37:LEU:N	1:B:37:LEU:CD1	2.75	0.49
1:A:88:GLU:C	1:A:89:PHE:HD2	2.15	0.49
1:C:119:VAL:HG13	1:C:150:PHE:CD1	2.48	0.49
1:D:140:LEU:HB3	1:D:144:MET:HE2	1.95	0.48
1:A:170:VAL:C	1:A:171:TRP:CE3	2.87	0.48
1:D:59:VAL:HG23	1:D:62:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:CD1	1:A:37:LEU:N	2.76	0.48
1:C:111:ARG:HH21	1:C:117:ILE:CD1	2.23	0.48
1:A:108:VAL:O	1:A:115:LEU:HD13	2.14	0.48
1:D:12:GLN:HG2	1:D:15:LYS:HB2	1.96	0.48
1:C:143:LEU:O	1:C:145:LYS:N	2.27	0.48
1:D:119:VAL:HG12	1:D:148:ASN:HD21	1.79	0.48
1:A:67:LEU:O	1:A:68:LEU:CD1	2.62	0.48
1:D:99:ASP:OD2	1:D:122:VAL:HG12	2.13	0.48
1:B:116:GLU:C	1:B:117:ILE:HD12	2.34	0.48
1:A:6:ARG:HB3	1:A:7:LYS:H	1.40	0.48
1:A:98:GLU:H	1:A:129:VAL:CG2	2.27	0.48
1:C:30:LEU:HD12	1:C:54:ASN:O	2.14	0.48
1:A:94:LYS:N	1:A:98:GLU:OE1	2.46	0.48
1:C:67:LEU:CD2	1:C:105:ARG:NH1	2.76	0.48
1:D:85:GLY:O	1:D:139:PRO:HA	2.13	0.48
1:B:91:ILE:CA	1:B:133:TRP:CZ3	2.97	0.48
1:A:135:HIS:ND1	1:A:136:VAL:N	2.61	0.47
1:B:46:ASN:O	1:B:46:ASN:CG	2.53	0.47
1:B:63:TRP:HZ3	1:B:65:ILE:HG22	1.78	0.47
1:A:119:VAL:HG22	1:A:143:LEU:HD23	1.96	0.47
1:D:140:LEU:HD13	1:D:144:MET:HE2	1.90	0.47
1:D:111:ARG:NH2	1:D:117:ILE:CG1	2.70	0.47
1:A:102:ILE:CG2	1:A:121:THR:HG23	2.44	0.47
1:C:50:THR:HG21	1:C:171:TRP:HB3	1.96	0.47
1:C:51:LEU:HD12	1:C:51:LEU:HA	1.47	0.47
1:A:6:ARG:HB3	1:A:8:LEU:HD22	1.97	0.47
1:B:130:THR:HB	1:B:132:ASP:HB2	1.95	0.47
1:B:106:ASP:OD1	1:B:117:ILE:N	2.37	0.47
1:B:169:THR:CG2	1:B:170:VAL:N	2.74	0.47
1:D:156:THR:O	1:D:157:CYS:HB3	2.15	0.47
1:B:168:PHE:CD1	1:B:168:PHE:C	2.88	0.47
1:C:39:VAL:CG1	1:C:39:VAL:O	2.63	0.47
1:C:78:LEU:O	1:C:79:SER:C	2.53	0.47
1:C:87:LEU:CD1	1:C:104:PHE:CZ	2.97	0.47
1:D:168:PHE:C	1:D:168:PHE:CD1	2.88	0.47
1:D:168:PHE:HD1	1:D:169:THR:CA	2.28	0.47
1:D:57:THR:HB	1:D:58:THR:H	1.43	0.47
1:A:55:VAL:O	1:A:56:GLN:C	2.53	0.47
1:B:68:LEU:HD12	1:B:158:LEU:HD23	1.96	0.47
1:D:9:LEU:O	1:D:81:TYR:OH	2.18	0.47
1:C:124:SER:OG	1:C:125:ASN:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:THR:HG23	1:C:37:LEU:N	2.30	0.46
1:B:37:LEU:HA	1:B:38:PRO:HD3	1.67	0.46
1:B:162:LYS:HD2	1:B:165:ALA:HA	1.96	0.46
1:A:7:LYS:H	1:A:8:LEU:HD22	1.79	0.46
1:D:110:GLU:CD	1:D:110:GLU:H	2.19	0.46
1:A:168:PHE:HD1	1:A:169:THR:O	1.98	0.46
1:B:179:SER:O	1:B:180:GLU:HB3	2.16	0.46
1:B:27:MET:HB2	1:B:27:MET:HE3	1.84	0.46
1:A:66:SER:O	1:A:159:VAL:HA	2.14	0.46
1:A:56:GLN:HB3	1:B:33:ILE:CD1	2.45	0.46
1:B:22:TRP:C	1:B:23:SER:OG	2.53	0.46
1:A:51:LEU:HB3	1:A:172:PHE:HB2	1.96	0.46
1:B:144:MET:SD	1:B:152:PRO:HB3	2.55	0.46
1:C:151:ASP:O	1:C:153:SER:N	2.49	0.46
1:C:102:ILE:HA	1:C:159:VAL:O	2.16	0.46
1:A:158:LEU:HG	1:A:159:VAL:N	2.31	0.46
1:D:147:ASN:OD1	1:D:147:ASN:N	2.49	0.46
1:C:54:ASN:HD22	1:C:169:THR:HG23	1.80	0.46
1:C:138:ILE:HA	1:C:139:PRO:HD2	1.38	0.46
1:A:121:THR:OG1	1:A:122:VAL:N	2.49	0.46
1:A:113:TYR:CD1	1:A:113:TYR:O	2.69	0.46
1:A:126:TYR:N	1:A:126:TYR:CD2	2.84	0.46
1:A:14:PHE:C	1:A:14:PHE:HD1	2.17	0.45
1:A:36:THR:HG23	1:A:37:LEU:O	2.16	0.45
1:B:23:SER:HB3	1:B:66:SER:OG	2.15	0.45
1:D:100:PHE:N	1:D:123:ILE:CD1	2.60	0.45
1:C:66:SER:O	1:C:159:VAL:HA	2.17	0.45
1:A:39:VAL:O	1:A:39:VAL:HG13	2.16	0.45
1:D:88:GLU:C	1:D:89:PHE:CD2	2.90	0.45
1:C:111:ARG:HG2	1:C:114:GLY:O	2.13	0.45
1:D:105:ARG:HG3	1:D:118:ASP:CG	2.37	0.45
1:C:121:THR:HG21	1:C:126:TYR:HE2	1.81	0.45
1:D:22:TRP:CZ3	1:D:24:GLY:N	2.84	0.45
1:A:23:SER:OG	1:A:37:LEU:CD1	2.64	0.45
1:A:51:LEU:CD1	1:A:52:ARG:N	2.77	0.45
1:B:156:THR:HG23	1:B:157:CYS:N	2.30	0.45
1:C:111:ARG:HE	1:C:117:ILE:HD11	1.81	0.45
1:C:22:TRP:HA	1:C:35:ASP:O	2.16	0.45
1:D:33:ILE:HD12	1:D:33:ILE:HA	1.27	0.45
1:D:91:ILE:C	1:D:91:ILE:CD1	2.77	0.45
1:C:148:ASN:ND2	1:C:148:ASN:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASP:C	1:A:153:SER:N	2.70	0.45
1:B:91:ILE:HA	1:B:133:TRP:CZ3	2.50	0.45
1:A:139:PRO:HG2	1:A:142:ASP:OD1	2.17	0.45
1:A:67:LEU:O	1:A:68:LEU:HD13	2.17	0.45
1:A:100:PHE:CD1	1:A:100:PHE:C	2.88	0.45
1:A:100:PHE:O	1:A:123:ILE:HD11	2.16	0.45
1:C:175:ILE:HG12	1:C:175:ILE:H	1.44	0.45
1:C:59:VAL:HG22	1:C:62:GLY:H	1.82	0.45
1:B:151:ASP:O	1:B:153:SER:N	2.50	0.45
1:B:8:LEU:HD22	1:B:179:SER:HB3	1.98	0.45
1:B:78:LEU:HD12	1:B:155:VAL:HG21	1.99	0.45
1:D:98:GLU:O	1:D:129:VAL:HG21	2.17	0.45
1:A:51:LEU:C	1:A:51:LEU:HD12	2.37	0.45
1:C:119:VAL:CG2	1:C:150:PHE:CE1	2.94	0.45
1:C:100:PHE:H	1:C:123:ILE:CD1	2.30	0.45
1:A:136:VAL:CG2	1:A:137:LYS:N	2.80	0.45
1:B:112:VAL:C	1:B:114:GLY:H	2.20	0.45
1:C:119:VAL:HG13	1:C:150:PHE:HD1	1.80	0.45
1:C:122:VAL:CG1	1:C:163:ARG:HD3	2.47	0.45
1:B:22:TRP:HA	1:B:35:ASP:O	2.17	0.45
1:A:98:GLU:N	1:A:129:VAL:HG21	2.32	0.45
1:A:66:SER:N	1:A:160:PHE:O	2.37	0.44
1:A:14:PHE:CD2	1:A:51:LEU:CD2	2.99	0.44
1:A:130:THR:O	1:A:132:ASP:N	2.47	0.44
1:A:80:GLN:HB3	1:A:80:GLN:HE21	1.63	0.44
1:A:46:ASN:O	1:A:46:ASN:CG	2.55	0.44
1:D:71:ARG:O	1:D:74:ASN:HB2	2.17	0.44
1:B:13:ILE:CG2	1:B:175:ILE:HB	2.45	0.44
1:D:155:VAL:H	1:D:155:VAL:HG23	1.51	0.44
1:A:14:PHE:CD1	1:A:15:LYS:N	2.86	0.44
1:D:48:LEU:HA	1:D:49:PRO:HD2	1.40	0.44
1:B:87:LEU:CD1	1:B:89:PHE:HD2	2.26	0.44
1:D:106:ASP:OD1	1:D:107:LYS:N	2.50	0.44
1:B:23:SER:OG	1:B:36:THR:HA	2.17	0.44
1:B:70:LEU:HD12	1:B:157:CYS:HA	2.00	0.44
1:C:125:ASN:HD22	1:C:125:ASN:N	2.14	0.44
1:A:68:LEU:O	1:A:157:CYS:CB	2.66	0.44
1:A:67:LEU:HA	1:A:67:LEU:HD23	1.51	0.44
1:C:53:LEU:HB3	1:C:170:VAL:HG23	1.99	0.44
1:D:19:VAL:O	1:D:36:THR:HG21	2.18	0.44
1:A:89:PHE:N	1:A:89:PHE:CD2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:THR:O	1:B:43:VAL:N	2.51	0.44
1:C:53:LEU:HB3	1:C:170:VAL:CG2	2.48	0.44
1:C:102:ILE:HG22	1:C:121:THR:O	2.18	0.44
1:B:40:ASP:OD2	1:B:41:THR:N	2.50	0.44
1:D:163:ARG:HD3	1:D:164:TYR:CD2	2.53	0.44
1:A:35:ASP:OD1	1:A:35:ASP:N	2.51	0.43
1:A:37:LEU:HD13	1:A:37:LEU:H	1.83	0.43
1:B:20:VAL:H	1:B:20:VAL:HG22	1.41	0.43
1:B:57:THR:HG22	1:B:58:THR:HG22	1.99	0.43
1:A:158:LEU:C	1:A:159:VAL:CG2	2.83	0.43
1:C:170:VAL:C	1:C:171:TRP:CE3	2.92	0.43
1:D:51:LEU:HA	1:D:51:LEU:HD12	1.84	0.43
1:B:14:PHE:CG	1:B:15:LYS:N	2.83	0.43
1:C:67:LEU:HD12	1:C:67:LEU:N	2.33	0.43
1:A:104:PHE:O	1:A:118:ASP:HA	2.19	0.43
1:B:92:LYS:HB2	1:B:133:TRP:CZ3	2.54	0.43
1:A:63:TRP:HZ3	1:A:65:ILE:HG22	1.83	0.43
1:D:91:ILE:CG1	1:D:170:VAL:CG2	2.97	0.43
1:D:170:VAL:HG23	1:D:171:TRP:H	1.84	0.43
1:B:22:TRP:CE3	1:B:23:SER:N	2.87	0.43
1:B:41:THR:C	1:B:43:VAL:N	2.69	0.43
1:A:87:LEU:HD13	1:A:177:ILE:HD13	2.01	0.43
1:B:146:ILE:C	1:B:148:ASN:H	2.05	0.43
1:A:111:ARG:NH2	1:A:117:ILE:HG13	2.33	0.43
1:A:115:LEU:HA	1:A:115:LEU:HD13	1.83	0.43
1:C:19:VAL:HG13	1:C:20:VAL:O	2.17	0.43
1:B:170:VAL:C	1:B:171:TRP:CE3	2.92	0.43
1:B:115:LEU:HD13	1:B:115:LEU:HA	1.68	0.43
1:B:67:LEU:HA	1:B:158:LEU:O	2.19	0.42
1:D:151:ASP:HA	1:D:152:PRO:HD3	1.76	0.42
1:A:19:VAL:HG23	1:A:36:THR:HG1	1.84	0.42
1:C:86:TYR:HA	1:C:140:LEU:HD23	2.01	0.42
1:D:36:THR:HG23	1:D:37:LEU:O	2.19	0.42
1:A:87:LEU:HD12	1:A:88:GLU:H	1.84	0.42
1:B:34:GLY:O	1:B:35:ASP:HB2	2.18	0.42
1:D:22:TRP:HZ3	1:D:65:ILE:HG23	1.84	0.42
1:C:127:VAL:CG1	1:C:134:GLN:HE21	2.29	0.42
1:C:89:PHE:CE1	1:C:91:ILE:HG21	2.53	0.42
1:B:39:VAL:HG23	1:B:40:ASP:N	2.32	0.42
1:C:39:VAL:O	1:C:39:VAL:HG13	2.20	0.42
1:D:103:GLY:C	1:D:104:PHE:CD2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:O	1:B:81:TYR:N	2.33	0.42
1:C:83:GLU:H	1:C:83:GLU:HG3	1.46	0.42
1:A:87:LEU:N	1:A:140:LEU:HD22	2.34	0.42
1:A:173:SER:C	1:A:175:ILE:HD12	2.39	0.42
1:D:99:ASP:OD2	1:D:123:ILE:HG12	2.19	0.42
1:A:101:VAL:CG1	1:A:102:ILE:H	2.33	0.42
1:C:126:TYR:HD2	1:C:126:TYR:N	2.16	0.42
1:B:51:LEU:HB3	1:B:172:PHE:HB2	2.02	0.42
1:D:33:ILE:C	1:D:35:ASP:N	2.70	0.42
1:B:102:ILE:HG13	1:B:160:PHE:CE2	2.55	0.42
1:C:121:THR:HG21	1:C:126:TYR:CE2	2.54	0.42
1:A:84:ASN:HA	1:A:84:ASN:HD22	1.73	0.42
1:D:141:ARG:HE	1:D:141:ARG:HB3	1.64	0.42
1:D:58:THR:HA	1:D:167:PRO:HD3	2.02	0.42
1:A:22:TRP:HA	1:A:35:ASP:O	2.20	0.42
1:A:71:ARG:O	1:A:74:ASN:N	2.46	0.42
1:C:175:ILE:HD12	1:C:175:ILE:HG23	1.53	0.42
1:C:104:PHE:O	1:C:118:ASP:HA	2.20	0.42
1:C:71:ARG:O	1:C:74:ASN:N	2.48	0.42
1:C:139:PRO:HG3	1:C:142:ASP:OD1	2.20	0.41
1:D:105:ARG:HG3	1:D:118:ASP:OD2	2.20	0.41
1:D:138:ILE:HA	1:D:139:PRO:HD2	1.52	0.41
1:B:37:LEU:HD12	1:B:37:LEU:HA	1.66	0.41
1:B:98:GLU:N	1:B:98:GLU:OE2	2.53	0.41
1:C:156:THR:O	1:C:157:CYS:HB3	2.20	0.41
1:D:82:VAL:HG13	1:D:83:GLU:CA	2.50	0.41
1:B:86:TYR:CG	1:B:137:LYS:HD2	2.55	0.41
1:A:12:GLN:OE1	1:A:176:LYS:HD2	2.21	0.41
1:D:91:ILE:CA	1:D:133:TRP:CZ3	2.99	0.41
1:A:163:ARG:HG3	1:A:164:TYR:N	2.35	0.41
1:C:143:LEU:C	1:C:145:LYS:N	2.71	0.41
1:D:117:ILE:HG22	1:D:118:ASP:H	1.83	0.41
1:C:127:VAL:HG11	1:C:134:GLN:HE21	1.82	0.41
1:A:128:THR:O	1:A:134:GLN:NE2	2.53	0.41
1:C:99:ASP:OD1	1:C:124:SER:HB3	2.20	0.41
1:A:166:ASP:HA	1:A:167:PRO:HD2	1.20	0.41
1:A:126:TYR:HE1	1:A:139:PRO:HG2	1.86	0.41
1:D:54:ASN:C	1:D:54:ASN:HD22	2.24	0.41
1:D:55:VAL:O	1:D:167:PRO:HB3	2.21	0.41
1:D:103:GLY:HA3	1:D:119:VAL:O	2.20	0.41
1:B:29:GLU:OE2	1:B:63:TRP:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:HD12	1:C:143:LEU:N	2.26	0.41
1:A:89:PHE:CG	1:A:175:ILE:HG13	2.55	0.41
1:B:103:GLY:O	1:B:158:LEU:HA	2.20	0.41
1:D:130:THR:HG23	1:D:132:ASP:O	2.21	0.41
1:D:72:GLY:O	1:D:73:TRP:CB	2.69	0.41
1:C:12:GLN:HA	1:C:12:GLN:OE1	2.19	0.41
1:D:87:LEU:N	1:D:140:LEU:HD21	2.35	0.41
1:D:91:ILE:CG1	1:D:170:VAL:HG21	2.51	0.41
1:A:22:TRP:CE3	1:A:23:SER:CA	3.03	0.41
1:D:99:ASP:C	1:D:123:ILE:HD11	2.40	0.41
1:B:94:LYS:HB2	1:B:169:THR:HB	2.02	0.41
1:D:104:PHE:HA	1:D:157:CYS:O	2.20	0.41
1:C:48:LEU:HB3	1:C:49:PRO:HD2	2.03	0.41
1:D:177:ILE:HD12	1:D:177:ILE:HG23	1.73	0.41
1:A:106:ASP:OD2	1:A:106:ASP:C	2.58	0.41
1:A:81:TYR:N	1:A:81:TYR:CD1	2.88	0.40
1:A:11:VAL:O	1:A:176:LYS:HA	2.21	0.40
1:A:20:VAL:HG21	1:C:18:PRO:CG	2.51	0.40
1:D:120:THR:O	1:D:120:THR:OG1	2.36	0.40
1:D:92:LYS:HB3	1:D:133:TRP:CE2	2.56	0.40
1:B:21:GLY:O	1:B:22:TRP:HB2	2.20	0.40
1:B:138:ILE:HA	1:B:139:PRO:HD2	1.70	0.40
1:A:126:TYR:HE1	1:A:139:PRO:CG	2.34	0.40
1:A:66:SER:HB3	1:A:160:PHE:HB2	2.02	0.40
1:D:111:ARG:HG2	1:D:113:TYR:CE2	2.56	0.40
1:B:92:LYS:HB2	1:B:133:TRP:CH2	2.57	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	173/205 (84%)	124 (72%)	36 (21%)	13 (8%)	1	15
1	B	172/205 (84%)	121 (70%)	34 (20%)	17 (10%)	1	10
1	C	171/205 (83%)	126 (74%)	35 (20%)	10 (6%)	2	23
1	D	171/205 (83%)	123 (72%)	31 (18%)	17 (10%)	1	10
All	All	687/820 (84%)	494 (72%)	136 (20%)	57 (8%)	1	13

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	SER
1	A	82	VAL
1	A	84	ASN
1	A	141	ARG
1	A	147	ASN
1	A	165	ALA
1	B	83	GLU
1	B	84	ASN
1	B	141	ARG
1	B	147	ASN
1	C	79	SER
1	C	84	ASN
1	C	141	ARG
1	C	147	ASN
1	D	42	THR
1	D	79	SER
1	D	84	ASN
1	D	141	ARG
1	D	147	ASN
1	A	26	GLY
1	B	26	GLY
1	B	56	GLN
1	B	79	SER
1	B	82	VAL
1	B	134	GLN
1	B	140	LEU
1	B	144	MET
1	C	26	GLY
1	C	56	GLN
1	D	26	GLY
1	D	46	ASN
1	D	56	GLN
1	D	82	VAL

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Mol	Chain	Res	Type
1	D	131	THR
1	D	134	GLN
1	A	16	ASP
1	A	89	PHE
1	A	131	THR
1	A	134	GLN
1	A	144	MET
1	B	27	MET
1	B	44	THR
1	C	134	GLN
1	C	144	MET
1	D	107	LYS
1	D	144	MET
1	B	61	SER
1	B	131	THR
1	D	16	ASP
1	A	7	LYS
1	B	42	THR
1	D	95	GLU
1	C	91	ILE
1	C	82	VAL
1	D	47	GLY
1	B	152	PRO
1	D	146	ILE

### 5.3.2 Protein sidechains [i](#)

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	159/182 (87%)	118 (74%)	41 (26%)	0	4
1	B	158/182 (87%)	114 (72%)	44 (28%)	0	3
1	C	157/182 (86%)	105 (67%)	52 (33%)	0	2
1	D	157/182 (86%)	93 (59%)	64 (41%)	0	1
All	All	631/728 (87%)	430 (68%)	201 (32%)	0	3

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	9	LEU
1	A	11	VAL
1	A	14	PHE
1	A	19	VAL
1	A	32	THR
1	A	35	ASP
1	A	36	THR
1	A	37	LEU
1	A	46	ASN
1	A	50	THR
1	A	51	LEU
1	A	54	ASN
1	A	55	VAL
1	A	57	THR
1	A	68	LEU
1	A	69	THR
1	A	71	ARG
1	A	75	THR
1	A	78	LEU
1	A	80	GLN
1	A	84	ASN
1	A	90	ASP
1	A	95	GLU
1	A	112	VAL
1	A	115	LEU
1	A	117	ILE
1	A	120	THR
1	A	121	THR
1	A	123	ILE
1	A	128	THR
1	A	129	VAL
1	A	132	ASP
1	A	142	ASP
1	A	146	ILE
1	A	157	CYS
1	A	161	SER
1	A	163	ARG
1	A	176	LYS
1	A	177	ILE
1	A	178	THR
1	B	8	LEU

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Mol	Chain	Res	Type
1	B	11	VAL
1	B	13	ILE
1	B	14	PHE
1	B	19	VAL
1	B	20	VAL
1	B	23	SER
1	B	25	SER
1	B	29	GLU
1	B	39	VAL
1	B	41	THR
1	B	42	THR
1	B	46	ASN
1	B	48	LEU
1	B	53	LEU
1	B	55	VAL
1	B	57	THR
1	B	61	SER
1	B	65	ILE
1	B	67	LEU
1	B	68	LEU
1	B	74	ASN
1	B	75	THR
1	B	80	GLN
1	B	84	ASN
1	B	87	LEU
1	B	101	VAL
1	B	112	VAL
1	B	115	LEU
1	B	119	VAL
1	B	120	THR
1	B	121	THR
1	B	122	VAL
1	B	123	ILE
1	B	127	VAL
1	B	131	THR
1	B	143	LEU
1	B	148	ASN
1	B	158	LEU
1	B	170	VAL
1	B	176	LYS
1	B	177	ILE
1	B	178	THR

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Mol	Chain	Res	Type
1	B	181	ASP
1	C	9	LEU
1	C	11	VAL
1	C	14	PHE
1	C	19	VAL
1	C	23	SER
1	C	25	SER
1	C	27	MET
1	C	32	THR
1	C	33	ILE
1	C	36	THR
1	C	37	LEU
1	C	41	THR
1	C	44	THR
1	C	50	THR
1	C	58	THR
1	C	67	LEU
1	C	71	ARG
1	C	75	THR
1	C	77	ASP
1	C	83	GLU
1	C	90	ASP
1	C	94	LYS
1	C	95	GLU
1	C	101	VAL
1	C	102	ILE
1	C	107	LYS
1	C	111	ARG
1	C	115	LEU
1	C	118	ASP
1	C	119	VAL
1	C	122	VAL
1	C	123	ILE
1	C	124	SER
1	C	126	TYR
1	C	127	VAL
1	C	128	THR
1	C	132	ASP
1	C	136	VAL
1	C	140	LEU
1	C	141	ARG
1	C	146	ILE

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Mol	Chain	Res	Type
1	C	148	ASN
1	C	152	PRO
1	C	153	SER
1	C	156	THR
1	C	162	LYS
1	C	163	ARG
1	C	166	ASP
1	C	169	THR
1	C	175	ILE
1	C	176	LYS
1	C	180	GLU
1	D	9	LEU
1	D	11	VAL
1	D	19	VAL
1	D	20	VAL
1	D	32	THR
1	D	33	ILE
1	D	35	ASP
1	D	36	THR
1	D	37	LEU
1	D	39	VAL
1	D	42	THR
1	D	50	THR
1	D	52	ARG
1	D	54	ASN
1	D	55	VAL
1	D	58	THR
1	D	59	VAL
1	D	60	GLN
1	D	61	SER
1	D	65	ILE
1	D	66	SER
1	D	71	ARG
1	D	77	ASP
1	D	79	SER
1	D	80	GLN
1	D	82	VAL
1	D	84	ASN
1	D	88	GLU
1	D	91	ILE
1	D	92	LYS
1	D	95	GLU

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Mol	Chain	Res	Type
1	D	98	GLU
1	D	99	ASP
1	D	101	VAL
1	D	105	ARG
1	D	112	VAL
1	D	113	TYR
1	D	116	GLU
1	D	120	THR
1	D	121	THR
1	D	122	VAL
1	D	123	ILE
1	D	124	SER
1	D	127	VAL
1	D	128	THR
1	D	130	THR
1	D	132	ASP
1	D	136	VAL
1	D	140	LEU
1	D	141	ARG
1	D	142	ASP
1	D	144	MET
1	D	146	ILE
1	D	147	ASN
1	D	154	SER
1	D	158	LEU
1	D	161	SER
1	D	163	ARG
1	D	166	ASP
1	D	170	VAL
1	D	173	SER
1	D	175	ILE
1	D	176	LYS
1	D	178	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	54	ASN
1	A	80	GLN
1	A	84	ASN
1	A	125	ASN

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Mol	Chain	Res	Type
1	A	135	HIS
1	B	54	ASN
1	B	74	ASN
1	B	80	GLN
1	B	125	ASN
1	B	148	ASN
1	C	54	ASN
1	C	80	GLN
1	C	125	ASN
1	C	134	GLN
1	C	135	HIS
1	C	148	ASN
1	D	12	GLN
1	D	54	ASN
1	D	56	GLN
1	D	60	GLN
1	D	84	ASN
1	D	135	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	175/205 (85%)	-0.70	0 <a href="#">100</a> <a href="#">100</a>	9, 36, 52, 62	4 (2%)
1	B	174/205 (84%)	-0.67	0 <a href="#">100</a> <a href="#">100</a>	10, 36, 52, 58	4 (2%)
1	C	173/205 (84%)	-0.69	0 <a href="#">100</a> <a href="#">100</a>	9, 36, 51, 57	4 (2%)
1	D	173/205 (84%)	-0.67	0 <a href="#">100</a> <a href="#">100</a>	10, 36, 51, 58	3 (1%)
All	All	695/820 (84%)	-0.68	0 <a href="#">100</a> <a href="#">100</a>	9, 36, 52, 62	15 (2%)

There are no RSRZ outliers to report.

### 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 carbohydrates 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.