



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:05 pm BST

PDB ID : 2ZE8  
Title : Crystal Structure of adenosine phosphate-isopentenyltransferase complexed with diphosphate  
Authors : Sakakibara, H.  
Deposited on : 2007-12-06  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

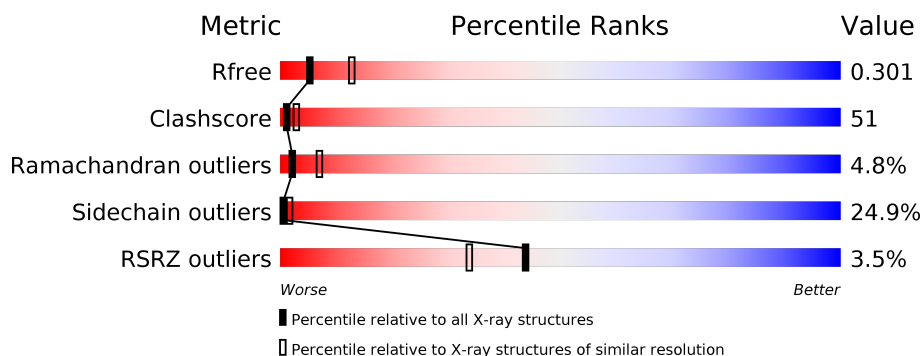
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	253	
1	B	253	
1	C	253	
1	D	253	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	POP	D	301	-	X	-	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7296 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 Isopentenyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1815	1146	327	333	9			
1	B	226	Total	C	N	O	S	0	0	0
			1815	1146	327	333	9			
1	C	226	Total	C	N	O	S	0	0	0
			1815	1146	327	333	9			
1	D	226	Total	C	N	O	S	0	0	0
			1815	1146	327	333	9			

There are 40 discrepancies between the modelled and reference sequences:

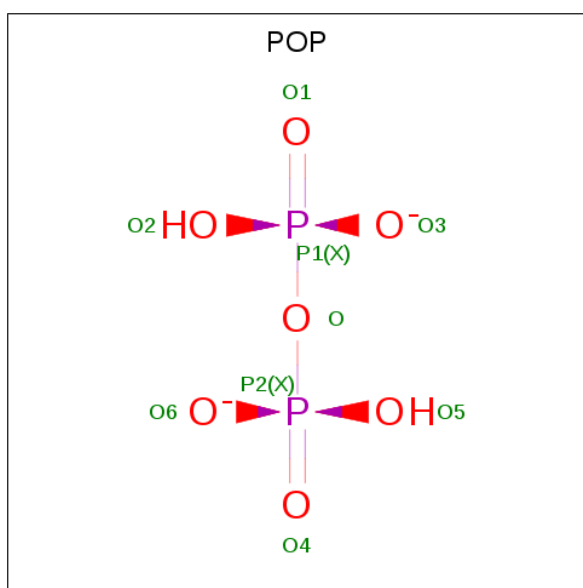
Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	EXPRESSION TAG	UNP P58758
A	245	SER	-	EXPRESSION TAG	UNP P58758
A	246	ARG	-	EXPRESSION TAG	UNP P58758
A	247	SER	-	EXPRESSION TAG	UNP P58758
A	248	HIS	-	EXPRESSION TAG	UNP P58758
A	249	HIS	-	EXPRESSION TAG	UNP P58758
A	250	HIS	-	EXPRESSION TAG	UNP P58758
A	251	HIS	-	EXPRESSION TAG	UNP P58758
A	252	HIS	-	EXPRESSION TAG	UNP P58758
A	253	HIS	-	EXPRESSION TAG	UNP P58758
B	244	GLY	-	EXPRESSION TAG	UNP P58758
B	245	SER	-	EXPRESSION TAG	UNP P58758
B	246	ARG	-	EXPRESSION TAG	UNP P58758
B	247	SER	-	EXPRESSION TAG	UNP P58758
B	248	HIS	-	EXPRESSION TAG	UNP P58758
B	249	HIS	-	EXPRESSION TAG	UNP P58758
B	250	HIS	-	EXPRESSION TAG	UNP P58758
B	251	HIS	-	EXPRESSION TAG	UNP P58758
B	252	HIS	-	EXPRESSION TAG	UNP P58758
B	253	HIS	-	EXPRESSION TAG	UNP P58758
C	244	GLY	-	EXPRESSION TAG	UNP P58758

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Chain	Residue	Modelled	Actual	Comment	Reference
C	245	SER	-	EXPRESSION TAG	UNP P58758
C	246	ARG	-	EXPRESSION TAG	UNP P58758
C	247	SER	-	EXPRESSION TAG	UNP P58758
C	248	HIS	-	EXPRESSION TAG	UNP P58758
C	249	HIS	-	EXPRESSION TAG	UNP P58758
C	250	HIS	-	EXPRESSION TAG	UNP P58758
C	251	HIS	-	EXPRESSION TAG	UNP P58758
C	252	HIS	-	EXPRESSION TAG	UNP P58758
C	253	HIS	-	EXPRESSION TAG	UNP P58758
D	244	GLY	-	EXPRESSION TAG	UNP P58758
D	245	SER	-	EXPRESSION TAG	UNP P58758
D	246	ARG	-	EXPRESSION TAG	UNP P58758
D	247	SER	-	EXPRESSION TAG	UNP P58758
D	248	HIS	-	EXPRESSION TAG	UNP P58758
D	249	HIS	-	EXPRESSION TAG	UNP P58758
D	250	HIS	-	EXPRESSION TAG	UNP P58758
D	251	HIS	-	EXPRESSION TAG	UNP P58758
D	252	HIS	-	EXPRESSION TAG	UNP P58758
D	253	HIS	-	EXPRESSION TAG	UNP P58758

- Molecule 2 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 9 7 2	0	0
2	B	1	Total O P 9 7 2	0	0

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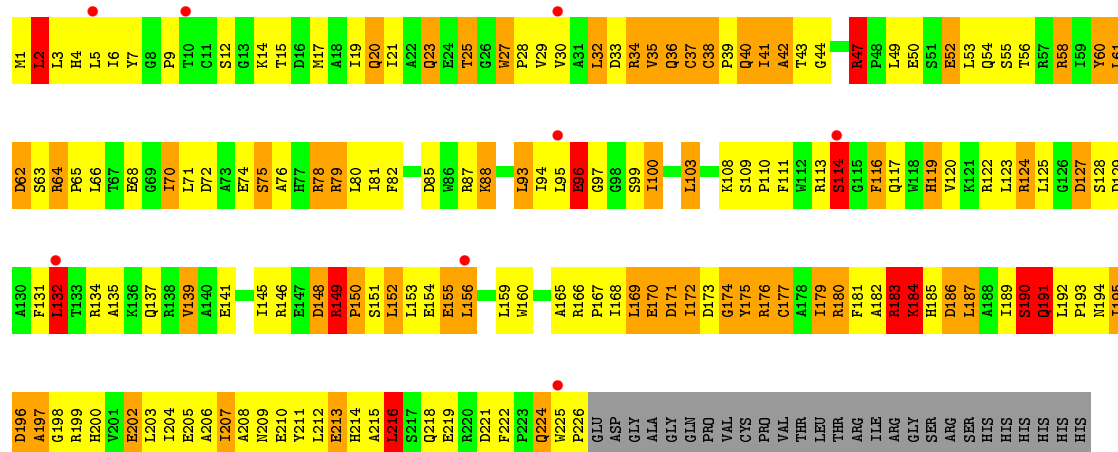
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	P	0	0
			9	7	2		
2	D	1	Total	O	P	0	0
			9	7	2		

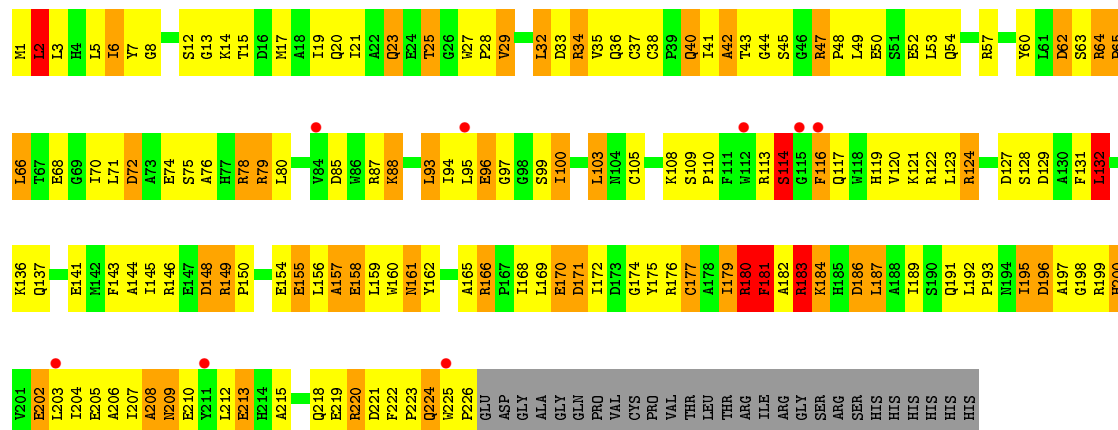


- Molecule 1: Isopentenyl transferase





• Molecule 1: Isopentenyl transferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.51Å 97.57Å 131.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	131.31 – 2.80 47.52 – 2.77	Depositor EDS
% Data completeness (in resolution range)	97.8 (131.31-2.80) 96.6 (47.52-2.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.230 , 0.302 0.231 , 0.301	Depositor DCC
$R_{free}$ test set	1594 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.8	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 90.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.459 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3713e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 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: POP

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	1.50	15/1856 (0.8%)	1.52	25/2514 (1.0%)
1	B	1.59	21/1856 (1.1%)	1.44	20/2514 (0.8%)
1	C	1.70	30/1856 (1.6%)	1.61	31/2514 (1.2%)
1	D	1.31	6/1856 (0.3%)	1.36	17/2514 (0.7%)
All	All	1.53	72/7424 (1.0%)	1.49	93/10056 (0.9%)

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	B	0	1
1	C	0	1
All	All	0	2

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	ASP	CG-OD1	11.22	1.51	1.25
1	C	183	ARG	CZ-NH1	10.84	1.47	1.33
1	B	177	CYS	CB-SG	-10.70	1.64	1.82
1	C	175	TYR	CD1-CE1	10.62	1.55	1.39
1	C	184	LYS	CE-NZ	10.05	1.74	1.49
1	C	186	ASP	CG-OD2	9.47	1.47	1.25
1	C	177	CYS	CB-SG	-9.35	1.66	1.82
1	B	50	GLU	CD-OE2	8.60	1.35	1.25
1	C	60	TYR	CZ-OH	8.55	1.52	1.37
1	B	60	TYR	CB-CG	-8.48	1.39	1.51
1	B	38	CYS	CB-SG	-8.05	1.68	1.82
1	C	183	ARG	CZ-NH2	7.97	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	GLU	CG-CD	7.62	1.63	1.51
1	D	105	CYS	CB-SG	-7.47	1.69	1.82
1	A	155	GLU	CG-CD	7.29	1.62	1.51
1	C	149	ARG	CG-CD	6.96	1.69	1.51
1	B	50	GLU	CG-CD	6.95	1.62	1.51
1	C	175	TYR	CE2-CZ	6.89	1.47	1.38
1	B	82	PHE	CE1-CZ	6.82	1.50	1.37
1	C	155	GLU	CG-CD	6.80	1.62	1.51
1	A	213	GLU	CB-CG	-6.74	1.39	1.52
1	C	60	TYR	N-CA	6.70	1.59	1.46
1	B	60	TYR	CZ-OH	6.55	1.49	1.37
1	C	139	VAL	CB-CG1	6.45	1.66	1.52
1	C	180	ARG	CG-CD	6.27	1.67	1.51
1	A	60	TYR	CD1-CE1	-6.27	1.29	1.39
1	B	59	ILE	CB-CG2	6.19	1.72	1.52
1	A	11	CYS	CB-SG	-6.17	1.71	1.82
1	C	184	LYS	CD-CE	6.16	1.66	1.51
1	B	105	CYS	CB-SG	-6.14	1.71	1.82
1	C	155	GLU	CD-OE2	6.04	1.32	1.25
1	C	211	TYR	CD2-CE2	-6.00	1.30	1.39
1	B	64	ARG	CG-CD	-5.98	1.37	1.51
1	B	82	PHE	CG-CD2	5.88	1.47	1.38
1	B	154	GLU	CG-CD	5.88	1.60	1.51
1	A	105	CYS	CB-SG	-5.83	1.72	1.81
1	A	59	ILE	CA-CB	-5.81	1.41	1.54
1	A	60	TYR	CD2-CE2	5.80	1.48	1.39
1	A	41	ILE	CB-CG2	-5.73	1.35	1.52
1	A	180	ARG	CZ-NH1	5.71	1.40	1.33
1	C	170	GLU	CG-CD	5.68	1.60	1.51
1	A	60	TYR	CB-CG	5.66	1.60	1.51
1	C	96	GLU	CB-CG	-5.61	1.41	1.52
1	D	181	PHE	CB-CG	5.54	1.60	1.51
1	A	207	ILE	CA-CB	-5.48	1.42	1.54
1	C	207	ILE	CA-CB	-5.45	1.42	1.54
1	D	177	CYS	CB-SG	-5.36	1.73	1.81
1	B	53	LEU	C-O	5.34	1.33	1.23
1	B	70	ILE	C-O	5.34	1.33	1.23
1	B	83	GLU	CD-OE1	5.32	1.31	1.25
1	D	37	CYS	CB-SG	-5.31	1.73	1.81
1	C	38	CYS	CA-CB	-5.31	1.42	1.53
1	D	180	ARG	CG-CD	5.31	1.65	1.51
1	B	60	TYR	CA-C	5.29	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	86	TRP	CB-CG	5.26	1.59	1.50
1	C	149	ARG	CZ-NH1	5.24	1.39	1.33
1	B	220	ARG	CZ-NH1	5.23	1.39	1.33
1	C	179	ILE	CB-CG2	5.22	1.69	1.52
1	C	180	ARG	CZ-NH1	5.17	1.39	1.33
1	A	59	ILE	CB-CG2	-5.16	1.36	1.52
1	B	68	GLU	CD-OE2	5.16	1.31	1.25
1	C	35	VAL	CB-CG2	-5.16	1.42	1.52
1	C	42	ALA	CA-CB	-5.14	1.41	1.52
1	C	183	ARG	CD-NE	5.14	1.55	1.46
1	B	154	GLU	CD-OE2	5.12	1.31	1.25
1	C	94	ILE	CA-CB	-5.12	1.43	1.54
1	A	81	ILE	CA-CB	-5.12	1.43	1.54
1	A	155	GLU	CD-OE2	5.05	1.31	1.25
1	C	30	VAL	CB-CG1	5.05	1.63	1.52
1	D	154	GLU	CG-CD	5.03	1.59	1.51
1	A	60	TYR	CE2-CZ	-5.01	1.32	1.38
1	C	27	TRP	CE3-CZ3	5.01	1.47	1.38

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	ASP	CB-CG-OD1	-12.32	107.21	118.30
1	C	183	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	B	64	ARG	NE-CZ-NH1	-11.36	114.62	120.30
1	A	93	LEU	CB-CG-CD1	-11.11	92.11	111.00
1	A	64	ARG	NE-CZ-NH1	-10.38	115.11	120.30
1	B	32	LEU	CA-CB-CG	-8.92	94.79	115.30
1	C	222	PHE	C-N-CD	8.85	146.99	128.40
1	D	64	ARG	NE-CZ-NH1	-8.54	116.03	120.30
1	B	105	CYS	CA-CB-SG	-8.44	98.81	114.00
1	D	32	LEU	CA-CB-CG	-8.44	95.89	115.30
1	C	155	GLU	N-CA-C	-8.42	88.27	111.00
1	D	93	LEU	CB-CG-CD1	-8.40	96.72	111.00
1	A	47	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	169	LEU	CB-CG-CD2	-7.96	97.48	111.00
1	C	64	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	A	32	LEU	CB-CG-CD2	-7.84	97.67	111.00
1	B	64	ARG	NE-CZ-NH2	7.81	124.20	120.30
1	A	149	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	C	32	LEU	CA-CB-CG	-7.62	97.78	115.30
1	C	159	LEU	CA-CB-CG	7.62	132.82	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	221	ASP	CB-CG-OD1	7.52	125.07	118.30
1	A	29	VAL	CB-CA-C	-7.26	97.60	111.40
1	C	93	LEU	CB-CG-CD1	-7.23	98.71	111.00
1	C	216	LEU	CA-CB-CG	-7.23	98.68	115.30
1	B	220	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	132	LEU	CA-CB-CG	7.00	131.41	115.30
1	B	78	ARG	CB-CA-C	6.97	124.34	110.40
1	C	47	ARG	CA-CB-CG	6.93	128.64	113.40
1	C	132	LEU	CA-CB-CG	6.87	131.09	115.30
1	A	60	TYR	CD1-CE1-CZ	6.85	125.97	119.80
1	A	32	LEU	CA-CB-CG	-6.68	99.94	115.30
1	D	132	LEU	CA-CB-CG	6.64	130.58	115.30
1	A	2	LEU	CB-CG-CD2	-6.62	99.75	111.00
1	D	186	ASP	C-N-CA	-6.50	105.46	121.70
1	B	52	GLU	N-CA-CB	6.46	122.22	110.60
1	B	53	LEU	CB-CG-CD2	-6.36	100.19	111.00
1	D	2	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	B	47	ARG	CA-CB-CG	6.26	127.17	113.40
1	D	29	VAL	CB-CA-C	-6.26	99.51	111.40
1	D	154	GLU	OE1-CD-OE2	-6.25	115.80	123.30
1	D	155	GLU	OE1-CD-OE2	-6.13	115.95	123.30
1	D	183	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	33	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	A	47	ARG	CA-CB-CG	6.07	126.75	113.40
1	A	58	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	132	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	149	ARG	CG-CD-NE	5.92	124.24	111.80
1	C	29	VAL	CB-CA-C	-5.91	100.17	111.40
1	C	79	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	B	166	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	D	78	ARG	CB-CA-C	5.81	122.02	110.40
1	D	79	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	172	ILE	CB-CA-C	-5.73	100.14	111.60
1	B	29	VAL	CB-CA-C	-5.71	100.56	111.40
1	A	5	LEU	CB-CG-CD1	-5.70	101.31	111.00
1	C	78	ARG	CB-CA-C	5.67	121.73	110.40
1	B	87	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	D	105	CYS	CA-CB-SG	-5.64	103.84	114.00
1	C	47	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	29	VAL	CG1-CB-CG2	5.62	119.89	110.90
1	C	169	LEU	CA-CB-CG	-5.58	102.47	115.30
1	D	166	ARG	NE-CZ-NH1	-5.53	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	LEU	N-CA-C	-5.50	96.16	111.00
1	B	32	LEU	CB-CG-CD1	5.48	120.31	111.00
1	B	93	LEU	CB-CA-C	-5.47	99.81	110.20
1	C	58	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	57	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	61	LEU	CB-CG-CD2	-5.39	101.84	111.00
1	D	32	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	C	47	ARG	CB-CA-C	-5.34	99.72	110.40
1	C	152	LEU	CA-CB-CG	5.33	127.57	115.30
1	C	222	PHE	C-N-CA	-5.32	99.65	122.00
1	C	52	GLU	N-CA-CB	5.32	120.18	110.60
1	A	155	GLU	N-CA-C	-5.27	96.77	111.00
1	A	212	LEU	CA-CB-CG	-5.25	103.23	115.30
1	A	78	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	17	MET	CG-SD-CE	5.24	108.59	100.20
1	A	80	LEU	CA-CB-CG	-5.23	103.27	115.30
1	C	175	TYR	CD1-CE1-CZ	-5.21	115.11	119.80
1	B	79	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	172	ILE	CG1-CB-CG2	5.17	122.78	111.40
1	A	159	LEU	CA-CB-CG	5.17	127.19	115.30
1	C	171	ASP	CB-CG-OD2	5.14	122.92	118.30
1	D	177	CYS	CA-CB-SG	-5.14	104.75	114.00
1	C	2	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	A	222	PHE	C-N-CD	5.08	139.07	128.40
1	B	95	LEU	CB-CG-CD1	-5.08	102.37	111.00
1	D	6	ILE	CB-CA-C	-5.04	101.51	111.60
1	B	47	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	169	LEU	CB-CG-CD1	5.02	119.53	111.00
1	A	166	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	B	60	TYR	CB-CG-CD1	-5.01	118.00	121.00
1	C	119	HIS	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	41	ILE	Peptide
1	C	190	SER	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	1815	0	1798	172	0
1	B	1815	0	1798	189	1
1	C	1815	0	1797	197	0
1	D	1815	0	1798	191	0
2	A	9	0	0	0	0
2	B	9	0	0	2	0
2	C	9	0	0	1	0
2	D	9	0	0	1	0
All	All	7296	0	7191	746	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 51.

All (746) 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:184:LYS:CE	1:C:184:LYS:NZ	1.74	1.48
1:B:176:ARG:HB3	1:B:176:ARG:NH1	1.38	1.38
1:B:176:ARG:CB	1:B:176:ARG:HH11	1.44	1.28
1:B:176:ARG:CB	1:B:176:ARG:NH1	2.07	1.12
1:C:34:ARG:HH11	1:C:34:ARG:HG2	1.15	1.11
1:D:149:ARG:HH11	1:D:149:ARG:HG3	0.99	1.11
1:A:183:ARG:HG3	1:A:183:ARG:HH11	1.11	1.08
1:C:183:ARG:HH11	1:C:183:ARG:HG3	1.00	1.08
1:C:49:LEU:CD2	1:C:149:ARG:HD3	1.84	1.07
1:C:187:LEU:HD12	1:C:187:LEU:N	1.69	1.07
1:C:183:ARG:HH11	1:C:183:ARG:CG	1.68	1.06
1:B:184:LYS:O	1:B:186:ASP:N	1.88	1.06
1:C:151:SER:OG	1:C:154:GLU:HG3	1.53	1.06
1:A:34:ARG:HH11	1:A:34:ARG:HG2	1.17	1.05
1:C:176:ARG:CB	1:C:176:ARG:HH11	1.69	1.05
1:C:183:ARG:NH1	1:C:183:ARG:HG3	1.73	1.02
1:D:21:ILE:O	1:D:25:THR:HB	1.59	1.01
1:C:187:LEU:HD12	1:C:187:LEU:H	0.89	1.01
1:C:25:THR:HG23	1:C:27:TRP:H	1.22	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:HH11	1:A:183:ARG:CG	1.75	1.00
1:B:209:ASN:H	1:B:209:ASN:HD22	1.07	1.00
1:C:224:GLN:N	1:C:224:GLN:HE21	1.58	0.99
1:C:187:LEU:H	1:C:187:LEU:CD1	1.75	0.98
1:C:166:ARG:O	1:C:170:GLU:HG3	1.65	0.97
1:A:61:LEU:HD21	1:A:80:LEU:HD13	1.45	0.97
1:A:187:LEU:H	1:A:187:LEU:HD12	1.30	0.97
1:A:151:SER:OG	1:A:154:GLU:HG3	1.63	0.96
1:D:224:GLN:HE21	1:D:224:GLN:N	1.62	0.96
1:D:149:ARG:HH11	1:D:149:ARG:CG	1.76	0.95
1:C:131:PHE:CD1	1:C:212:LEU:HD13	2.01	0.95
1:A:161:ASN:H	1:A:161:ASN:HD22	1.02	0.94
1:C:176:ARG:HH11	1:C:176:ARG:HB3	1.32	0.94
1:D:199:ARG:HA	1:D:202:GLU:OE2	1.67	0.94
1:D:113:ARG:O	1:D:114:SER:HB3	1.66	0.94
1:D:209:ASN:HD22	1:D:209:ASN:N	1.66	0.94
1:A:49:LEU:HD21	1:A:149:ARG:HH11	1.32	0.94
1:A:25:THR:CG2	1:A:27:TRP:H	1.80	0.94
1:A:36:GLN:O	1:A:47:ARG:NH1	2.01	0.94
1:B:21:ILE:O	1:B:25:THR:HB	1.69	0.93
1:C:160:TRP:CZ2	1:C:166:ARG:HD3	2.05	0.92
1:D:149:ARG:HG3	1:D:149:ARG:NH1	1.82	0.92
1:A:25:THR:HG23	1:A:27:TRP:H	1.35	0.92
1:A:21:ILE:O	1:A:25:THR:HB	1.69	0.91
1:C:131:PHE:HD1	1:C:212:LEU:HD13	1.33	0.91
1:A:113:ARG:O	1:A:114:SER:HB3	1.69	0.91
1:C:49:LEU:HD21	1:C:149:ARG:CD	2.01	0.90
1:D:161:ASN:HD22	1:D:161:ASN:H	1.19	0.90
1:A:99:SER:O	1:A:103:LEU:HD12	1.72	0.90
1:B:113:ARG:O	1:B:114:SER:HB3	1.70	0.90
1:D:136:LYS:HE2	1:D:205:GLU:HG3	1.54	0.90
1:B:100:ILE:HD11	1:B:218:GLN:HA	1.54	0.90
1:A:49:LEU:HD21	1:A:149:ARG:NH1	1.87	0.89
1:C:47:ARG:HD2	1:C:60:TYR:CZ	2.07	0.89
1:A:131:PHE:CD1	1:A:212:LEU:HD13	2.08	0.89
1:D:34:ARG:HG2	1:D:34:ARG:HH11	1.38	0.89
1:C:160:TRP:CE2	1:C:166:ARG:HD3	2.09	0.88
1:A:53:LEU:O	1:A:54:GLN:HB2	1.73	0.87
1:D:25:THR:HG23	1:D:27:TRP:H	1.40	0.87
1:A:173:ASP:OD1	1:A:176:ARG:NH2	2.06	0.87
1:D:99:SER:O	1:D:103:LEU:HD12	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLU:O	1:B:209:ASN:ND2	2.08	0.87
1:A:161:ASN:ND2	1:A:161:ASN:H	1.70	0.87
1:C:113:ARG:O	1:C:114:SER:HB3	1.73	0.87
1:D:181:PHE:CD1	1:D:203:LEU:HD13	2.10	0.87
1:C:25:THR:CG2	1:C:27:TRP:H	1.88	0.86
1:B:183:ARG:HH11	1:B:183:ARG:CG	1.89	0.86
1:B:172:ILE:O	1:B:173:ASP:O	1.91	0.86
1:B:25:THR:HG23	1:B:27:TRP:CG	2.12	0.85
1:C:34:ARG:HG2	1:C:34:ARG:NH1	1.84	0.85
1:D:32:LEU:HD11	1:D:95:LEU:HB3	1.58	0.85
1:A:166:ARG:O	1:A:170:GLU:HG3	1.77	0.85
1:C:219:GLU:OE2	1:C:219:GLU:HA	1.75	0.85
1:B:192:LEU:N	1:B:193:PRO:CD	2.39	0.84
1:C:176:ARG:NH1	1:C:176:ARG:HB2	1.92	0.84
1:C:23:GLN:NE2	1:C:54:GLN:HB3	1.92	0.84
1:C:131:PHE:CD1	1:C:212:LEU:CD1	2.61	0.84
1:A:183:ARG:NH1	1:A:183:ARG:HG3	1.88	0.84
1:C:99:SER:O	1:C:103:LEU:HD12	1.78	0.84
1:D:183:ARG:HG2	1:D:183:ARG:HH11	1.39	0.84
1:C:15:THR:O	1:C:19:ILE:HG13	1.77	0.83
1:C:176:ARG:HH11	1:C:176:ARG:HB2	1.44	0.83
1:C:151:SER:OG	1:C:154:GLU:CG	2.27	0.83
1:A:34:ARG:HG2	1:A:34:ARG:NH1	1.86	0.83
1:D:25:THR:CG2	1:D:27:TRP:H	1.91	0.83
1:C:49:LEU:HD21	1:C:149:ARG:HD3	1.55	0.83
1:C:44:GLY:HA3	1:C:175:TYR:OH	1.80	0.82
1:C:176:ARG:NH1	1:C:176:ARG:CB	2.42	0.82
1:B:189:ILE:O	1:B:191:GLN:N	2.11	0.82
1:B:224:GLN:HE21	1:B:224:GLN:N	1.77	0.81
1:B:25:THR:HG23	1:B:27:TRP:H	1.42	0.81
1:D:36:GLN:O	1:D:47:ARG:NH1	2.14	0.81
1:B:145:ILE:O	1:B:146:ARG:HG3	1.80	0.81
1:A:50:GLU:O	1:A:53:LEU:HB2	1.80	0.81
1:C:21:ILE:O	1:C:25:THR:HB	1.81	0.81
1:B:100:ILE:CD1	1:B:218:GLN:HA	2.10	0.81
1:B:32:LEU:HD11	1:B:95:LEU:HB3	1.62	0.81
1:C:189:ILE:HA	1:C:192:LEU:CD1	2.11	0.81
1:B:209:ASN:N	1:B:209:ASN:HD22	1.78	0.80
1:C:173:ASP:O	1:C:175:TYR:N	2.14	0.80
1:D:146:ARG:HD3	1:D:149:ARG:NH1	1.97	0.80
1:B:224:GLN:N	1:B:224:GLN:NE2	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:NH1	1:C:71:LEU:O	2.15	0.80
1:D:1:MET:O	1:D:116:PHE:HB3	1.81	0.80
1:B:34:ARG:HH11	1:B:34:ARG:HG2	1.47	0.79
1:C:151:SER:CB	1:C:154:GLU:HG3	2.11	0.79
1:A:23:GLN:NE2	1:A:54:GLN:HB3	1.97	0.79
1:C:203:LEU:HD12	1:C:203:LEU:O	1.82	0.79
1:B:44:GLY:HA3	1:B:175:TYR:OH	1.82	0.79
1:B:44:GLY:HA2	1:B:152:LEU:HD12	1.63	0.78
1:A:136:LYS:HE2	1:A:205:GLU:HG3	1.65	0.78
1:A:131:PHE:CE1	1:A:212:LEU:HA	2.19	0.77
1:C:176:ARG:NH1	1:C:210:GLU:OE1	2.17	0.77
1:C:23:GLN:HE22	1:C:54:GLN:HB3	1.48	0.77
1:B:120:VAL:HG21	1:B:225:TRP:CD1	2.19	0.77
1:B:210:GLU:O	1:B:213:GLU:HB3	1.84	0.77
1:C:135:ALA:O	1:C:139:VAL:HG23	1.83	0.77
1:B:183:ARG:HH11	1:B:183:ARG:HG3	1.50	0.77
1:B:99:SER:O	1:B:103:LEU:HD12	1.84	0.77
1:C:120:VAL:HG21	1:C:225:TRP:CD1	2.20	0.77
1:D:145:ILE:O	1:D:146:ARG:HG3	1.85	0.77
1:A:161:ASN:N	1:A:161:ASN:HD22	1.83	0.77
1:B:223:PRO:C	1:B:224:GLN:HE21	1.87	0.76
1:A:176:ARG:NH1	1:A:210:GLU:CD	2.39	0.76
1:D:195:ILE:HD12	1:D:196:ASP:OD2	1.85	0.76
1:C:189:ILE:HA	1:C:192:LEU:HD11	1.68	0.76
1:C:196:ASP:O	1:C:198:GLY:N	2.18	0.76
1:D:146:ARG:HD3	1:D:149:ARG:CZ	2.16	0.76
1:C:205:GLU:O	1:C:209:ASN:ND2	2.19	0.75
1:D:176:ARG:HB3	1:D:176:ARG:NH1	2.02	0.75
1:A:156:LEU:HD13	1:A:175:TYR:HD2	1.50	0.75
1:D:34:ARG:NH1	1:D:71:LEU:O	2.19	0.75
1:B:7:TYR:CE2	1:B:122:ARG:HD2	2.22	0.74
1:B:5:LEU:HD12	1:B:6:ILE:N	2.01	0.74
1:D:161:ASN:ND2	1:D:161:ASN:H	1.85	0.74
1:D:5:LEU:HD12	1:D:6:ILE:N	2.02	0.74
1:A:1:MET:O	1:A:116:PHE:HB3	1.87	0.74
1:C:75:SER:O	1:C:76:ALA:C	2.26	0.74
1:D:176:ARG:HH11	1:D:176:ARG:HB3	1.52	0.74
1:A:187:LEU:N	1:A:187:LEU:HD12	2.00	0.73
1:D:7:TYR:CE2	1:D:122:ARG:HD2	2.23	0.73
1:A:161:ASN:N	1:A:161:ASN:ND2	2.35	0.73
1:A:23:GLN:HE22	1:A:54:GLN:HB3	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:LEU:O	1:D:215:ALA:HB3	1.89	0.73
1:D:123:LEU:HD23	1:D:123:LEU:N	2.02	0.73
1:D:131:PHE:CE1	1:D:212:LEU:HA	2.24	0.73
1:D:219:GLU:OE2	1:D:219:GLU:HA	1.87	0.73
1:B:161:ASN:H	1:B:161:ASN:HD22	1.36	0.73
1:B:183:ARG:HG3	1:B:183:ARG:NH1	2.03	0.72
1:C:173:ASP:OD1	1:C:176:ARG:NH2	2.19	0.72
1:D:224:GLN:NE2	1:D:224:GLN:H	1.87	0.72
1:D:224:GLN:NE2	1:D:224:GLN:N	2.36	0.72
1:B:23:GLN:NE2	1:B:54:GLN:HB3	2.03	0.72
1:B:2:LEU:O	1:B:3:LEU:HD23	1.88	0.72
1:C:204:ILE:O	1:C:205:GLU:C	2.22	0.72
1:C:2:LEU:O	1:C:3:LEU:HD23	1.90	0.72
1:C:50:GLU:O	1:C:53:LEU:HB2	1.90	0.72
1:D:149:ARG:CG	1:D:149:ARG:NH1	2.42	0.72
1:C:120:VAL:HG21	1:C:225:TRP:HD1	1.55	0.71
1:D:224:GLN:HE21	1:D:224:GLN:H	1.36	0.71
1:B:185:HIS:HB2	1:B:187:LEU:HD11	1.71	0.71
1:B:184:LYS:C	1:B:186:ASP:H	1.94	0.71
1:B:209:ASN:H	1:B:209:ASN:ND2	1.86	0.71
1:C:43:THR:HB	1:C:155:GLU:OE1	1.90	0.71
1:D:5:LEU:HD12	1:D:6:ILE:H	1.54	0.71
1:C:25:THR:HG23	1:C:27:TRP:N	2.04	0.70
1:D:44:GLY:HA3	1:D:175:TYR:OH	1.91	0.70
1:C:137:GLN:NE2	1:C:141:GLU:OE1	2.22	0.70
1:A:49:LEU:CD2	1:A:149:ARG:HH11	2.04	0.70
1:D:148:ASP:N	1:D:148:ASP:OD2	2.24	0.70
1:D:184:LYS:HE3	1:D:184:LYS:HA	1.74	0.70
1:B:195:ILE:O	1:B:196:ASP:C	2.28	0.70
1:D:209:ASN:ND2	1:D:209:ASN:N	2.37	0.70
1:B:15:THR:O	1:B:19:ILE:HG13	1.90	0.70
1:B:122:ARG:C	1:B:123:LEU:HD23	2.11	0.70
1:B:1:MET:O	1:B:116:PHE:HB3	1.90	0.70
1:B:223:PRO:C	1:B:224:GLN:NE2	2.45	0.70
1:C:176:ARG:NH1	1:C:210:GLU:CD	2.45	0.70
1:B:165:ALA:O	1:B:169:LEU:HB2	1.91	0.70
1:A:137:GLN:NE2	1:A:141:GLU:OE1	2.23	0.69
1:D:195:ILE:C	1:D:195:ILE:HD12	2.12	0.69
1:C:23:GLN:HE22	1:C:54:GLN:CB	2.05	0.69
1:D:23:GLN:NE2	1:D:54:GLN:HB3	2.06	0.69
1:A:173:ASP:O	1:A:175:TYR:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ILE:C	1:B:191:GLN:H	1.95	0.69
1:A:32:LEU:HD11	1:A:95:LEU:HB3	1.73	0.69
1:A:5:LEU:HD12	1:A:6:ILE:H	1.58	0.69
1:C:189:ILE:O	1:C:192:LEU:HD12	1.92	0.69
1:D:120:VAL:HG21	1:D:225:TRP:CD1	2.28	0.69
1:B:204:ILE:O	1:B:205:GLU:C	2.27	0.69
1:B:192:LEU:N	1:B:193:PRO:HD2	2.07	0.68
1:B:224:GLN:HE21	1:B:224:GLN:CA	2.06	0.68
1:B:25:THR:CG2	1:B:27:TRP:H	2.07	0.68
1:D:179:ILE:O	1:D:182:ALA:N	2.24	0.68
1:D:191:GLN:HA	1:D:191:GLN:NE2	2.08	0.68
1:D:195:ILE:CG2	1:D:200:HIS:HD2	2.06	0.68
1:D:32:LEU:HB2	1:D:97:GLY:HA3	1.73	0.68
1:B:28:PRO:HG2	1:B:93:LEU:HD23	1.74	0.68
1:C:100:ILE:HD11	1:C:218:GLN:HA	1.75	0.68
1:D:204:ILE:O	1:D:208:ALA:HB2	1.94	0.68
1:C:34:ARG:NH1	1:C:34:ARG:CG	2.57	0.68
1:D:25:THR:HG23	1:D:27:TRP:CG	2.29	0.68
1:C:145:ILE:O	1:C:146:ARG:HG3	1.94	0.68
1:C:32:LEU:HD11	1:C:95:LEU:HB3	1.75	0.67
1:C:183:ARG:CG	1:C:183:ARG:NH1	2.38	0.67
1:D:172:ILE:HG22	1:D:175:TYR:HD1	1.59	0.67
1:C:190:SER:O	1:C:191:GLN:NE2	2.26	0.67
1:B:209:ASN:N	1:B:209:ASN:ND2	2.42	0.67
1:A:49:LEU:CD2	1:A:149:ARG:NH1	2.58	0.67
1:D:50:GLU:O	1:D:53:LEU:HB2	1.95	0.66
1:B:123:LEU:N	1:B:123:LEU:HD23	2.08	0.66
1:B:176:ARG:HB2	1:B:176:ARG:NH1	2.05	0.66
1:C:123:LEU:HD23	1:C:123:LEU:N	2.11	0.66
1:A:5:LEU:HD12	1:A:6:ILE:N	2.09	0.66
1:C:58:ARG:HD3	1:C:60:TYR:OH	1.96	0.66
1:D:218:GLN:O	1:D:222:PHE:CD1	2.49	0.66
1:A:148:ASP:N	1:A:148:ASP:OD2	2.26	0.66
1:A:34:ARG:NH1	1:A:71:LEU:O	2.29	0.66
1:B:176:ARG:HH11	1:B:176:ARG:HB3	0.56	0.66
1:D:34:ARG:NH1	1:D:34:ARG:HG2	2.08	0.65
1:A:23:GLN:HE22	1:A:54:GLN:CB	2.09	0.65
1:D:181:PHE:HZ	1:D:199:ARG:HG2	1.61	0.65
1:A:7:TYR:CE2	1:A:122:ARG:HD2	2.31	0.65
1:C:187:LEU:CD1	1:C:187:LEU:N	2.42	0.65
1:A:75:SER:O	1:A:76:ALA:C	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ARG:C	1:C:123:LEU:HD23	2.17	0.65
1:C:34:ARG:O	1:C:37:CYS:HB2	1.96	0.65
1:A:28:PRO:HG2	1:A:93:LEU:CD2	2.26	0.65
1:A:47:ARG:HD2	1:A:60:TYR:CZ	2.32	0.64
1:D:199:ARG:O	1:D:200:HIS:C	2.36	0.64
1:D:172:ILE:CG2	1:D:175:TYR:HD1	2.11	0.64
1:A:176:ARG:HH11	1:A:210:GLU:CD	2.01	0.64
1:A:34:ARG:HH11	1:A:34:ARG:CG	1.97	0.64
1:D:122:ARG:C	1:D:123:LEU:HD23	2.16	0.64
1:D:15:THR:O	1:D:19:ILE:HG13	1.98	0.64
1:B:47:ARG:HD2	1:B:60:TYR:CZ	2.32	0.64
1:D:87:ARG:HD3	1:D:93:LEU:HD21	1.79	0.64
1:C:49:LEU:CD2	1:C:149:ARG:CD	2.62	0.63
1:C:5:LEU:HD12	1:C:6:ILE:N	2.13	0.63
1:A:207:ILE:O	1:A:208:ALA:C	2.36	0.63
1:B:34:ARG:HG2	1:B:34:ARG:NH1	2.13	0.63
1:A:100:ILE:HD11	1:A:218:GLN:HA	1.80	0.63
1:A:15:THR:O	1:A:19:ILE:HG13	1.97	0.63
1:B:136:LYS:HE2	1:B:205:GLU:HG3	1.78	0.63
1:C:132:LEU:HD11	1:C:212:LEU:HD22	1.81	0.63
1:C:7:TYR:CE2	1:C:122:ARG:HD2	2.34	0.63
1:D:202:GLU:O	1:D:206:ALA:N	2.32	0.63
1:D:218:GLN:HB3	1:D:222:PHE:CE1	2.34	0.63
1:B:34:ARG:NH1	1:B:71:LEU:O	2.32	0.63
1:D:145:ILE:C	1:D:146:ARG:HG3	2.19	0.63
1:A:25:THR:HG23	1:A:27:TRP:N	2.11	0.62
1:A:62:ASP:HB2	1:A:79:ARG:NH1	2.14	0.62
1:B:170:GLU:O	1:B:176:ARG:HG3	2.00	0.62
1:C:219:GLU:OE2	1:C:219:GLU:CA	2.39	0.62
1:A:123:LEU:N	1:A:123:LEU:HD23	2.14	0.62
1:A:106:MET:HB3	1:A:225:TRP:HH2	1.65	0.62
1:A:145:ILE:O	1:A:146:ARG:HG3	2.00	0.62
1:D:179:ILE:O	1:D:180:ARG:C	2.37	0.62
1:D:183:ARG:CG	1:D:183:ARG:HH11	2.12	0.62
1:B:28:PRO:HG2	1:B:93:LEU:CD2	2.30	0.62
1:A:25:THR:HG22	1:A:27:TRP:H	1.62	0.61
1:B:185:HIS:HB2	1:B:187:LEU:CD1	2.30	0.61
1:D:144:ALA:O	1:D:149:ARG:NH2	2.33	0.61
1:A:219:GLU:HA	1:A:219:GLU:OE2	1.99	0.61
1:C:210:GLU:O	1:C:213:GLU:HB3	2.01	0.61
1:D:75:SER:O	1:D:76:ALA:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:ASP:O	1:D:88:LYS:HG3	1.99	0.61
1:A:85:ASP:O	1:A:88:LYS:HG3	2.00	0.61
1:D:162:TYR:O	1:D:165:ALA:HB3	2.00	0.61
1:B:32:LEU:HB2	1:B:97:GLY:HA3	1.83	0.61
1:A:225:TRP:O	1:A:226:PRO:O	2.19	0.61
1:A:23:GLN:HE22	1:A:54:GLN:HG3	1.64	0.61
1:B:148:ASP:N	1:B:148:ASP:OD2	2.31	0.61
1:B:160:TRP:CZ2	1:B:166:ARG:HD3	2.36	0.61
1:D:70:ILE:HD11	1:D:172:ILE:HD11	1.83	0.61
1:D:149:ARG:HD2	1:D:150:PRO:O	2.00	0.60
1:D:156:LEU:HD21	1:D:189:ILE:HG23	1.84	0.60
1:C:81:ILE:HG22	1:C:82:PHE:N	2.16	0.60
1:D:218:GLN:O	1:D:222:PHE:HD1	1.84	0.60
1:B:25:THR:CG2	1:B:27:TRP:HB2	2.32	0.60
1:C:23:GLN:HE22	1:C:54:GLN:CG	2.15	0.60
1:D:195:ILE:O	1:D:196:ASP:C	2.40	0.60
1:C:44:GLY:HA3	1:C:175:TYR:HH	1.67	0.60
1:C:148:ASP:OD2	1:C:148:ASP:N	2.28	0.59
1:C:49:LEU:HD21	1:C:149:ARG:NE	2.18	0.59
1:C:9:PRO:HB3	1:C:215:ALA:HB1	1.83	0.59
1:D:177:CYS:HB2	1:D:210:GLU:OE1	2.02	0.59
1:D:132:LEU:HD12	1:D:209:ASN:ND2	2.17	0.59
1:D:2:LEU:O	1:D:3:LEU:HD23	2.02	0.59
1:A:195:ILE:O	1:A:195:ILE:HG23	2.02	0.59
1:C:207:ILE:HG22	1:C:208:ALA:N	2.18	0.59
1:D:162:TYR:N	1:D:162:TYR:CD2	2.70	0.59
1:A:23:GLN:HE22	1:A:54:GLN:CG	2.15	0.59
1:C:156:LEU:HG	1:C:189:ILE:HG21	1.84	0.59
1:C:191:GLN:N	1:C:193:PRO:HD2	2.18	0.59
1:D:23:GLN:HE22	1:D:54:GLN:HB3	1.67	0.59
1:C:28:PRO:HG2	1:C:93:LEU:CD2	2.33	0.58
1:D:35:VAL:HG22	1:D:70:ILE:HD12	1.84	0.58
1:A:61:LEU:HD21	1:A:80:LEU:CD1	2.27	0.58
1:D:1:MET:HE3	1:D:116:PHE:HD2	1.68	0.58
1:D:220:ARG:HG2	1:D:221:ASP:OD1	2.03	0.58
1:A:209:ASN:HD22	1:A:209:ASN:N	2.01	0.58
1:A:87:ARG:HD3	1:A:93:LEU:HD21	1.84	0.58
1:C:25:THR:HG23	1:C:27:TRP:CG	2.39	0.58
1:A:34:ARG:HG2	1:A:71:LEU:O	2.04	0.57
1:B:179:ILE:HG22	1:B:179:ILE:O	2.03	0.57
1:D:2:LEU:HD12	1:D:3:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LEU:N	1:D:193:PRO:HD2	2.20	0.57
1:B:1:MET:HE3	1:B:116:PHE:HD2	1.70	0.57
1:D:199:ARG:HG3	1:D:202:GLU:OE2	2.05	0.57
1:B:192:LEU:H	1:B:193:PRO:CD	2.18	0.57
1:C:152:LEU:O	1:C:156:LEU:HB2	2.04	0.57
1:A:128:SER:O	1:A:129:ASP:C	2.43	0.57
1:A:25:THR:HG23	1:A:27:TRP:CG	2.40	0.57
1:A:61:LEU:O	1:A:79:ARG:HD3	2.05	0.57
1:B:146:ARG:HD3	1:B:149:ARG:CZ	2.35	0.57
1:B:5:LEU:HD12	1:B:6:ILE:H	1.69	0.57
1:C:1:MET:O	1:C:116:PHE:HB3	2.05	0.57
1:B:33:ASP:CG	1:B:36:GLN:HB2	2.26	0.56
1:B:145:ILE:C	1:B:146:ARG:HG3	2.26	0.56
1:D:161:ASN:N	1:D:161:ASN:ND2	2.52	0.56
1:B:25:THR:CG2	1:B:27:TRP:CG	2.87	0.56
1:C:179:ILE:O	1:C:182:ALA:HB3	2.05	0.56
1:D:181:PHE:CD1	1:D:203:LEU:CD1	2.86	0.56
1:B:224:GLN:CA	1:B:224:GLN:NE2	2.68	0.56
1:C:173:ASP:HA	1:C:176:ARG:HH12	1.69	0.56
1:C:184:LYS:CD	1:C:184:LYS:NZ	2.65	0.56
1:C:87:ARG:HD3	1:C:93:LEU:HD21	1.86	0.56
1:D:53:LEU:O	1:D:54:GLN:HB2	2.06	0.56
1:A:100:ILE:CD1	1:A:218:GLN:HA	2.35	0.56
1:A:135:ALA:O	1:A:139:VAL:HG23	2.05	0.56
1:A:81:ILE:HG22	1:A:82:PHE:N	2.14	0.56
1:B:160:TRP:CE2	1:B:166:ARG:HD3	2.41	0.56
1:D:176:ARG:CB	1:D:176:ARG:NH1	2.69	0.56
1:B:213:GLU:O	1:B:216:LEU:HB2	2.06	0.55
1:A:145:ILE:C	1:A:146:ARG:HG3	2.26	0.55
1:B:10:THR:HG22	1:B:215:ALA:HB2	1.89	0.55
1:C:189:ILE:HA	1:C:192:LEU:HD12	1.87	0.55
1:A:122:ARG:C	1:A:123:LEU:HD23	2.27	0.55
1:D:42:ALA:HA	1:D:47:ARG:HG3	1.87	0.55
1:B:53:LEU:O	1:B:56:THR:OG1	2.14	0.55
1:B:87:ARG:HD3	1:B:93:LEU:HD21	1.88	0.55
1:C:100:ILE:CD1	1:C:218:GLN:HA	2.36	0.55
1:D:122:ARG:NH2	1:D:219:GLU:OE2	2.40	0.55
1:D:42:ALA:HA	1:D:47:ARG:CG	2.37	0.55
1:A:35:VAL:HG12	1:A:35:VAL:O	2.04	0.54
1:B:145:ILE:O	1:B:146:ARG:CG	2.54	0.54
1:B:169:LEU:C	1:B:171:ASP:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:PHE:CD1	1:D:65:PRO:HG3	2.42	0.54
1:D:145:ILE:O	1:D:146:ARG:CG	2.56	0.54
1:A:1:MET:HE3	1:A:116:PHE:HD2	1.73	0.54
1:B:215:ALA:HA	1:B:218:GLN:HG3	1.89	0.54
1:C:61:LEU:O	1:C:79:ARG:HD3	2.07	0.54
1:B:172:ILE:C	1:B:173:ASP:O	2.46	0.54
1:C:185:HIS:HB2	1:C:187:LEU:HD11	1.90	0.54
1:D:192:LEU:N	1:D:193:PRO:CD	2.70	0.54
1:C:23:GLN:HE22	1:C:54:GLN:HG3	1.72	0.54
1:A:125:LEU:HD22	1:A:215:ALA:HB1	1.89	0.54
1:B:183:ARG:HH11	1:B:183:ARG:HG2	1.73	0.54
1:B:189:ILE:C	1:B:191:GLN:N	2.58	0.54
1:C:191:GLN:HA	1:C:191:GLN:NE2	2.22	0.54
1:C:53:LEU:O	1:C:54:GLN:HB2	2.06	0.54
1:B:224:GLN:HE21	1:B:224:GLN:HA	1.72	0.54
1:B:50:GLU:O	1:B:53:LEU:HB2	2.07	0.54
1:C:23:GLN:NE2	1:C:54:GLN:CB	2.67	0.53
1:D:175:TYR:O	1:D:179:ILE:HD12	2.09	0.53
1:C:209:ASN:HD22	1:C:209:ASN:H	1.56	0.53
1:C:189:ILE:C	1:C:192:LEU:HD12	2.28	0.53
1:D:1:MET:HE3	1:D:116:PHE:CD2	2.43	0.53
1:D:181:PHE:CZ	1:D:199:ARG:HG2	2.42	0.53
1:D:183:ARG:NH1	1:D:183:ARG:CG	2.71	0.53
1:B:204:ILE:O	1:B:207:ILE:N	2.41	0.53
1:C:224:GLN:H	1:C:224:GLN:HE21	1.48	0.53
1:B:72:ASP:C	1:B:72:ASP:OD2	2.47	0.53
1:C:139:VAL:HG21	1:C:207:ILE:HG22	1.91	0.53
1:C:1:MET:HE3	1:C:116:PHE:HD2	1.74	0.53
1:D:100:ILE:CD1	1:D:218:GLN:HA	2.39	0.53
1:A:158:GLU:O	1:A:161:ASN:ND2	2.41	0.52
1:C:160:TRP:CD2	1:C:189:ILE:HG13	2.45	0.52
1:D:160:TRP:CE3	1:D:166:ARG:HG2	2.44	0.52
1:B:169:LEU:O	1:B:171:ASP:N	2.43	0.52
1:D:137:GLN:NE2	1:D:141:GLU:OE1	2.36	0.52
1:D:179:ILE:CG2	1:D:183:ARG:NH1	2.73	0.52
1:D:195:ILE:CD1	1:D:196:ASP:OD2	2.56	0.52
1:D:2:LEU:HD12	1:D:3:LEU:N	2.23	0.52
1:C:85:ASP:O	1:C:88:LYS:HG3	2.08	0.52
1:B:180:ARG:O	1:B:181:PHE:C	2.48	0.52
1:C:32:LEU:HB2	1:C:97:GLY:HA3	1.91	0.52
1:A:183:ARG:NH1	1:A:183:ARG:CG	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ILE:HA	1:D:155:GLU:OE2	2.09	0.52
1:A:28:PRO:HG2	1:A:93:LEU:HD23	1.89	0.52
1:D:100:ILE:HD11	1:D:218:GLN:HA	1.92	0.52
1:D:207:ILE:O	1:D:210:GLU:N	2.40	0.52
1:B:35:VAL:HG12	1:B:35:VAL:O	2.10	0.52
1:D:33:ASP:OD1	1:D:35:VAL:N	2.43	0.52
1:B:169:LEU:C	1:B:171:ASP:N	2.63	0.52
1:B:1:MET:HE3	1:B:116:PHE:CD2	2.44	0.52
1:C:34:ARG:HG2	1:C:71:LEU:O	2.10	0.51
1:C:47:ARG:HD2	1:C:60:TYR:OH	2.09	0.51
1:D:35:VAL:HG12	1:D:35:VAL:O	2.09	0.51
1:D:49:LEU:CD1	1:D:146:ARG:NH2	2.73	0.51
1:A:49:LEU:N	1:A:52:GLU:HG2	2.25	0.51
1:C:184:LYS:CG	1:C:184:LYS:NZ	2.73	0.51
1:C:35:VAL:HG22	1:C:70:ILE:HD12	1.92	0.51
1:C:132:LEU:CD1	1:C:212:LEU:HD22	2.40	0.51
1:D:181:PHE:O	1:D:181:PHE:CD1	2.64	0.51
1:B:155:GLU:O	1:B:159:LEU:HB2	2.11	0.51
1:A:181:PHE:CD1	1:A:203:LEU:HD13	2.45	0.51
1:B:183:ARG:CG	1:B:183:ARG:NH1	2.56	0.51
1:C:47:ARG:CD	1:C:60:TYR:CZ	2.88	0.51
1:A:49:LEU:CD1	1:A:146:ARG:NH2	2.74	0.51
1:A:131:PHE:HE1	1:A:212:LEU:HA	1.72	0.51
1:D:62:ASP:HB2	1:D:79:ARG:NH1	2.25	0.51
1:C:189:ILE:CA	1:C:192:LEU:HD12	2.40	0.51
1:C:145:ILE:C	1:C:146:ARG:HG3	2.30	0.51
1:B:75:SER:O	1:B:76:ALA:C	2.50	0.51
1:D:169:LEU:C	1:D:171:ASP:H	2.13	0.51
1:C:125:LEU:HD22	1:C:215:ALA:HB3	1.94	0.50
1:C:180:ARG:O	1:C:181:PHE:C	2.49	0.50
1:C:28:PRO:HG2	1:C:93:LEU:HD23	1.91	0.50
1:C:6:ILE:O	1:C:96:GLU:HA	2.11	0.50
1:D:179:ILE:O	1:D:181:PHE:N	2.44	0.50
1:D:28:PRO:HG2	1:D:93:LEU:CD2	2.40	0.50
1:D:28:PRO:HG2	1:D:93:LEU:HD23	1.93	0.50
1:C:54:GLN:O	1:C:55:SER:HB2	2.11	0.50
1:A:204:ILE:O	1:A:205:GLU:C	2.49	0.50
1:B:15:THR:HA	1:B:96:GLU:OE1	2.10	0.50
1:B:161:ASN:H	1:B:161:ASN:ND2	2.07	0.50
1:B:195:ILE:O	1:B:196:ASP:O	2.29	0.50
1:B:25:THR:CG2	1:B:27:TRP:CB	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:O	1:B:79:ARG:HD3	2.11	0.50
1:B:75:SER:O	1:B:77:HIS:N	2.44	0.50
1:B:32:LEU:CD1	1:B:95:LEU:HB3	2.38	0.50
1:D:161:ASN:N	1:D:161:ASN:HD22	1.99	0.50
1:A:2:LEU:O	1:A:3:LEU:HD23	2.10	0.50
1:A:42:ALA:N	1:A:155:GLU:OE2	2.45	0.50
1:C:156:LEU:HG	1:C:189:ILE:CG2	2.40	0.50
1:D:225:TRP:O	1:D:226:PRO:C	2.50	0.50
1:C:62:ASP:OD1	1:C:64:ARG:HD2	2.11	0.50
1:B:81:ILE:O	1:B:85:ASP:N	2.40	0.50
1:C:53:LEU:O	1:C:56:THR:OG1	2.23	0.50
1:A:224:GLN:H	1:A:224:GLN:HE21	1.58	0.49
1:B:209:ASN:O	1:B:212:LEU:HB3	2.12	0.49
1:C:195:ILE:O	1:C:197:ALA:N	2.45	0.49
1:C:36:GLN:O	1:C:47:ARG:NH1	2.38	0.49
1:A:155:GLU:O	1:A:159:LEU:HB2	2.12	0.49
1:A:182:ALA:HB2	1:A:192:LEU:HD11	1.93	0.49
1:B:36:GLN:O	1:B:47:ARG:NH1	2.40	0.49
1:B:65:PRO:O	1:B:66:LEU:C	2.48	0.49
1:B:38:CYS:O	1:B:41:ILE:HG13	2.12	0.49
1:C:149:ARG:CG	1:C:149:ARG:HH11	2.26	0.49
1:B:25:THR:HG23	1:B:27:TRP:CB	2.41	0.49
1:D:143:PHE:CE2	1:D:203:LEU:HD23	2.46	0.49
1:D:25:THR:HG22	1:D:27:TRP:H	1.75	0.49
1:C:189:ILE:CA	1:C:192:LEU:CD1	2.89	0.49
1:D:14:LYS:HZ1	2:D:301:POP:P2	2.36	0.49
1:A:191:GLN:HA	1:A:191:GLN:NE2	2.28	0.48
1:C:214:HIS:O	1:C:218:GLN:HG3	2.12	0.48
1:D:156:LEU:CD2	1:D:189:ILE:HG23	2.43	0.48
1:D:174:GLY:HA2	1:D:207:ILE:HG23	1.95	0.48
1:D:191:GLN:CA	1:D:191:GLN:NE2	2.72	0.48
1:A:132:LEU:HD21	1:A:212:LEU:HD22	1.94	0.48
1:A:220:ARG:HG2	1:A:221:ASP:OD1	2.13	0.48
1:B:21:ILE:O	1:B:25:THR:CB	2.53	0.48
1:D:181:PHE:HE2	1:D:202:GLU:HB2	1.78	0.48
1:A:156:LEU:CD2	1:A:189:ILE:CG2	2.92	0.48
1:B:19:ILE:O	1:B:23:GLN:HB2	2.14	0.48
1:C:131:PHE:CE1	1:C:212:LEU:HA	2.49	0.48
1:A:214:HIS:O	1:A:215:ALA:C	2.52	0.48
1:C:128:SER:O	1:C:129:ASP:C	2.50	0.48
1:C:5:LEU:HD12	1:C:6:ILE:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ALA:O	1:D:158:GLU:C	2.50	0.48
1:B:162:TYR:CD2	1:B:162:TYR:N	2.80	0.48
1:D:32:LEU:HB2	1:D:97:GLY:CA	2.42	0.48
1:A:50:GLU:HA	1:A:53:LEU:HD12	1.95	0.48
1:B:224:GLN:O	1:B:226:PRO:HD2	2.14	0.48
1:A:185:HIS:HB2	1:A:187:LEU:HD11	1.96	0.48
1:A:86:TRP:O	1:A:86:TRP:CE3	2.67	0.48
1:B:176:ARG:NH1	1:B:210:GLU:OE1	2.46	0.48
1:B:2:LEU:HD12	1:B:3:LEU:H	1.79	0.48
1:D:149:ARG:C	1:D:150:PRO:O	2.45	0.48
1:A:212:LEU:O	1:A:215:ALA:HB3	2.13	0.48
1:B:204:ILE:O	1:B:206:ALA:N	2.47	0.48
1:C:199:ARG:HA	1:C:202:GLU:HG3	1.96	0.48
1:C:35:VAL:HA	1:C:70:ILE:CD1	2.43	0.48
1:D:38:CYS:O	1:D:41:ILE:HG13	2.13	0.48
1:A:120:VAL:HG21	1:A:225:TRP:CD1	2.49	0.47
1:B:32:LEU:HA	1:B:32:LEU:HD23	1.38	0.47
1:C:184:LYS:HB2	1:C:184:LYS:HE3	1.81	0.47
1:D:192:LEU:HB2	1:D:193:PRO:HD3	1.96	0.47
1:D:203:LEU:O	1:D:207:ILE:HG13	2.14	0.47
1:D:47:ARG:HB3	1:D:60:TYR:OH	2.14	0.47
1:B:225:TRP:HA	1:B:226:PRO:HD2	1.50	0.47
1:B:32:LEU:HB2	1:B:97:GLY:CA	2.43	0.47
1:D:209:ASN:O	1:D:212:LEU:HB3	2.14	0.47
1:D:48:PRO:HB2	1:D:52:GLU:HG3	1.96	0.47
1:B:50:GLU:OE1	1:D:57:ARG:NE	2.48	0.47
1:D:169:LEU:C	1:D:171:ASP:N	2.68	0.47
1:D:94:ILE:O	1:D:95:LEU:HD23	2.15	0.47
1:B:85:ASP:O	1:B:87:ARG:N	2.48	0.47
1:D:143:PHE:HE2	1:D:203:LEU:HD23	1.80	0.47
1:A:202:GLU:O	1:A:206:ALA:N	2.49	0.46
1:B:75:SER:HA	1:B:78:ARG:HH11	1.79	0.46
1:C:124:ARG:HH11	1:C:124:ARG:CG	2.28	0.46
1:C:72:ASP:OD2	1:C:72:ASP:C	2.53	0.46
1:D:23:GLN:HE22	1:D:54:GLN:CB	2.28	0.46
1:A:157:ALA:O	1:A:158:GLU:C	2.53	0.46
1:B:181:PHE:O	1:B:184:LYS:HB3	2.16	0.46
1:A:156:LEU:HD23	1:A:189:ILE:HG22	1.98	0.46
1:A:106:MET:HB3	1:A:225:TRP:CH2	2.48	0.46
1:B:23:GLN:HE22	1:B:54:GLN:CG	2.28	0.46
1:B:96:GLU:OE2	1:B:97:GLY:HA2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:LEU:H	1:D:52:GLU:CG	2.28	0.46
1:A:192:LEU:HA	1:A:192:LEU:HD23	1.57	0.46
1:D:65:PRO:O	1:D:66:LEU:C	2.53	0.46
1:B:85:ASP:O	1:B:88:LYS:HG3	2.15	0.46
1:B:9:PRO:HB3	1:B:215:ALA:HB1	1.98	0.46
1:B:124:ARG:HH11	1:B:124:ARG:CG	2.28	0.46
1:B:75:SER:C	1:B:77:HIS:N	2.68	0.46
1:C:177:CYS:SG	1:C:207:ILE:HG13	2.55	0.46
1:C:207:ILE:O	1:C:208:ALA:C	2.53	0.46
1:D:176:ARG:NH1	1:D:210:GLU:CD	2.69	0.46
1:A:156:LEU:HD13	1:A:175:TYR:CD2	2.41	0.46
1:A:34:ARG:O	1:A:37:CYS:HB2	2.16	0.46
1:C:1:MET:HE3	1:C:116:PHE:CD2	2.51	0.46
1:B:33:ASP:OD1	1:B:33:ASP:C	2.54	0.46
1:B:139:VAL:O	1:B:140:ALA:C	2.55	0.45
1:B:204:ILE:HG22	1:B:205:GLU:N	2.31	0.45
1:B:34:ARG:CG	1:B:34:ARG:NH1	2.80	0.45
1:C:99:SER:O	1:C:103:LEU:CD1	2.58	0.45
1:B:82:PHE:CE1	1:D:65:PRO:HG3	2.52	0.45
1:C:145:ILE:HG22	1:C:146:ARG:N	2.31	0.45
1:C:204:ILE:O	1:C:206:ALA:N	2.49	0.45
1:A:177:CYS:HB2	1:A:210:GLU:CD	2.37	0.45
1:B:205:GLU:O	1:B:206:ALA:C	2.54	0.45
1:B:23:GLN:HE22	1:B:54:GLN:HB3	1.76	0.45
1:C:39:PRO:HB3	1:C:47:ARG:NH2	2.31	0.45
1:A:61:LEU:O	1:A:62:ASP:CB	2.65	0.45
1:B:65:PRO:HB2	1:B:68:GLU:HG2	1.98	0.45
1:A:147:GLU:HG3	1:A:147:GLU:H	1.60	0.45
1:A:17:MET:O	1:A:20:GLN:HB2	2.16	0.45
1:A:33:ASP:OD1	1:A:33:ASP:C	2.55	0.45
1:D:177:CYS:HB2	1:D:210:GLU:CD	2.35	0.45
1:B:22:ALA:HA	1:B:25:THR:HG22	1.98	0.45
1:A:4:HIS:CE1	1:A:21:ILE:HD13	2.51	0.45
1:B:161:ASN:ND2	1:B:161:ASN:N	2.63	0.45
1:B:6:ILE:O	1:B:96:GLU:HA	2.16	0.45
1:C:127:ASP:O	1:C:128:SER:C	2.54	0.45
1:D:109:SER:HA	1:D:110:PRO:HD3	1.72	0.45
1:D:34:ARG:HH12	1:D:72:ASP:HA	1.82	0.45
1:A:1:MET:HE3	1:A:116:PHE:CD2	2.51	0.45
1:A:47:ARG:HD2	1:A:60:TYR:OH	2.15	0.45
1:A:49:LEU:H	1:A:52:GLU:HG2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ALA:HB2	1:C:192:LEU:HD21	1.99	0.45
1:D:49:LEU:H	1:D:52:GLU:HG2	1.82	0.45
1:A:14:LYS:O	1:A:17:MET:HB2	2.17	0.45
1:B:75:SER:O	1:B:78:ARG:N	2.50	0.45
1:D:182:ALA:O	1:D:186:ASP:N	2.50	0.45
1:B:25:THR:HG21	1:B:27:TRP:HB2	1.98	0.45
1:A:212:LEU:HA	1:A:212:LEU:HD12	1.68	0.44
1:B:146:ARG:HD3	1:B:149:ARG:NE	2.32	0.44
1:B:8:GLY:O	1:B:14:LYS:HE2	2.17	0.44
1:B:29:VAL:HA	1:B:94:ILE:HB	1.99	0.44
1:A:149:ARG:HA	1:A:150:PRO:HD2	1.80	0.44
1:B:175:TYR:O	1:B:178:ALA:HB3	2.16	0.44
1:C:131:PHE:CD1	1:C:212:LEU:HD12	2.49	0.44
1:D:196:ASP:CG	1:D:196:ASP:O	2.55	0.44
1:D:225:TRP:HA	1:D:226:PRO:HD2	1.76	0.44
1:A:173:ASP:HA	1:A:176:ARG:HH22	1.83	0.44
1:A:66:LEU:HA	1:A:66:LEU:HD22	1.78	0.44
1:B:74:GLU:HA	1:B:74:GLU:OE1	2.17	0.44
1:A:195:ILE:HG23	1:A:200:HIS:HD2	1.81	0.44
1:B:106:MET:HA	1:B:112:TRP:CD1	2.53	0.44
1:C:153:LEU:HA	1:C:153:LEU:HD23	1.72	0.44
1:A:41:ILE:C	1:A:155:GLU:OE2	2.56	0.44
1:A:195:ILE:O	1:A:196:ASP:O	2.34	0.44
1:A:225:TRP:HA	1:A:226:PRO:HD2	1.73	0.44
1:B:44:GLY:HA2	1:B:152:LEU:CD1	2.39	0.44
1:C:65:PRO:HB2	1:C:68:GLU:HG2	2.00	0.44
1:A:131:PHE:HD1	1:A:212:LEU:HD13	1.76	0.44
1:B:3:LEU:HA	1:B:3:LEU:HD23	1.71	0.44
1:C:131:PHE:HA	1:C:134:ARG:NH1	2.33	0.44
1:C:61:LEU:O	1:C:62:ASP:CB	2.64	0.44
1:C:96:GLU:OE2	1:C:97:GLY:HA2	2.17	0.44
1:D:29:VAL:HA	1:D:94:ILE:HB	2.00	0.44
1:A:131:PHE:HA	1:A:134:ARG:NH1	2.32	0.44
1:A:5:LEU:HD12	1:A:95:LEU:O	2.18	0.44
1:C:9:PRO:HB3	1:C:215:ALA:CB	2.48	0.44
1:D:183:ARG:HG2	1:D:183:ARG:NH1	2.16	0.44
1:D:207:ILE:O	1:D:208:ALA:C	2.56	0.44
1:A:132:LEU:CD2	1:A:212:LEU:HD22	2.48	0.44
1:A:109:SER:HA	1:A:110:PRO:HD3	1.64	0.43
1:B:62:ASP:HB2	1:B:79:ARG:NH1	2.33	0.43
1:C:225:TRP:HA	1:C:226:PRO:HD2	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:VAL:C	1:C:37:CYS:H	2.22	0.43
1:D:191:GLN:HE21	1:D:191:GLN:CA	2.31	0.43
1:A:172:ILE:HG22	1:A:173:ASP:O	2.18	0.43
1:A:32:LEU:HA	1:A:32:LEU:HD23	1.17	0.43
1:C:38:CYS:O	1:C:41:ILE:HG13	2.18	0.43
1:C:49:LEU:H	1:C:52:GLU:HG2	1.82	0.43
1:D:8:GLY:O	1:D:14:LYS:HE2	2.18	0.43
1:D:34:ARG:NH1	1:D:34:ARG:CG	2.75	0.43
1:D:40:GLN:HB3	1:D:40:GLN:HE21	1.56	0.43
1:B:27:TRP:N	1:B:27:TRP:CD1	2.85	0.43
1:B:137:GLN:NE2	1:B:141:GLU:OE1	2.35	0.43
1:B:131:PHE:CE1	1:B:212:LEU:HA	2.54	0.43
1:B:36:GLN:HG3	1:B:45:SER:O	2.19	0.43
1:D:43:THR:OG1	1:D:149:ARG:HD3	2.17	0.43
1:A:124:ARG:CG	1:A:124:ARG:HH11	2.32	0.43
1:A:156:LEU:HD12	1:A:169:LEU:HD13	2.01	0.43
1:A:219:GLU:OE2	1:A:219:GLU:CA	2.62	0.43
1:B:207:ILE:O	1:B:210:GLU:HB3	2.18	0.43
1:A:35:VAL:HG22	1:A:70:ILE:HD12	2.01	0.43
1:B:176:ARG:CB	1:B:176:ARG:CZ	2.80	0.43
1:B:53:LEU:O	1:B:54:GLN:HB2	2.18	0.43
1:C:145:ILE:CG2	1:C:146:ARG:N	2.82	0.43
1:B:127:ASP:O	1:B:128:SER:C	2.57	0.43
1:C:34:ARG:HH12	1:C:72:ASP:HA	1.84	0.43
1:D:14:LYS:O	1:D:15:THR:C	2.57	0.43
1:B:200:HIS:O	1:B:203:LEU:HB3	2.19	0.43
1:B:23:GLN:NE2	1:B:54:GLN:CB	2.78	0.43
1:B:47:ARG:HB3	1:B:60:TYR:OH	2.19	0.43
1:C:214:HIS:C	1:C:216:LEU:N	2.68	0.43
1:D:80:LEU:HA	1:D:80:LEU:HD12	1.61	0.43
1:A:176:ARG:HH12	1:A:210:GLU:CD	2.19	0.43
1:B:34:ARG:O	1:B:37:CYS:HB2	2.19	0.43
1:C:153:LEU:O	1:C:156:LEU:HB3	2.19	0.43
1:C:61:LEU:HD23	1:C:61:LEU:HA	1.76	0.43
1:D:131:PHE:CE1	1:D:212:LEU:CA	3.00	0.43
1:B:81:ILE:HG12	1:B:111:PHE:CD2	2.54	0.42
1:C:40:GLN:H	1:C:40:GLN:HG2	1.64	0.42
1:A:29:VAL:HA	1:A:94:ILE:HB	2.01	0.42
1:A:36:GLN:HA	1:A:45:SER:OG	2.19	0.42
1:B:34:ARG:HH12	1:B:72:ASP:HA	1.84	0.42
1:C:32:LEU:HD23	1:C:32:LEU:HA	1.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:PHE:CE1	1:D:203:LEU:HD13	2.53	0.42
1:A:78:ARG:O	1:A:81:ILE:HB	2.20	0.42
1:B:109:SER:HA	1:B:110:PRO:HD3	1.66	0.42
1:B:14:LYS:HZ1	2:B:301:POP:P2	2.42	0.42
1:B:44:GLY:HA3	1:B:175:TYR:CZ	2.52	0.42
1:C:14:LYS:NZ	2:C:301:POP:O	2.42	0.42
1:D:7:TYR:CZ	1:D:122:ARG:HD2	2.53	0.42
1:D:195:ILE:O	1:D:195:ILE:HG23	2.19	0.42
1:D:6:ILE:O	1:D:96:GLU:HA	2.19	0.42
1:A:153:LEU:HD22	1:A:192:LEU:HB3	2.01	0.42
1:B:191:GLN:NE2	1:B:191:GLN:HA	2.34	0.42
1:C:212:LEU:HD12	1:C:212:LEU:HA	1.67	0.42
1:C:125:LEU:HD22	1:C:215:ALA:CB	2.49	0.42
1:C:80:LEU:HA	1:C:80:LEU:HD12	1.78	0.42
1:D:210:GLU:O	1:D:213:GLU:HB3	2.19	0.42
1:A:137:GLN:O	1:A:141:GLU:HG3	2.18	0.42
1:D:13:GLY:O	1:D:17:MET:HG3	2.20	0.42
1:D:169:LEU:O	1:D:171:ASP:N	2.52	0.42
1:D:176:ARG:CZ	1:D:176:ARG:CB	2.97	0.42
1:A:48:PRO:HB2	1:A:52:GLU:HG3	2.02	0.42
1:A:80:LEU:HA	1:A:80:LEU:HD12	1.78	0.42
1:C:170:GLU:O	1:C:176:ARG:HG3	2.19	0.42
1:D:70:ILE:HG22	1:D:71:LEU:N	2.34	0.42
1:A:195:ILE:CG2	1:A:200:HIS:HD2	2.33	0.42
1:B:7:TYR:CZ	1:B:122:ARG:HD2	2.55	0.42
1:B:195:ILE:HD12	1:B:196:ASP:N	2.35	0.42
1:C:49:LEU:HD23	1:C:149:ARG:HD3	1.88	0.42
1:A:7:TYR:CZ	1:A:122:ARG:HD2	2.55	0.42
1:B:23:GLN:HE22	1:B:54:GLN:HG3	1.85	0.42
1:C:166:ARG:O	1:C:167:PRO:C	2.53	0.42
1:C:4:HIS:CE1	1:C:21:ILE:HD13	2.55	0.42
1:C:44:GLY:HA3	1:C:175:TYR:CZ	2.52	0.42
1:C:49:LEU:N	1:C:52:GLU:HG2	2.35	0.42
1:A:204:ILE:O	1:A:206:ALA:N	2.53	0.42
1:C:224:GLN:NE2	1:C:224:GLN:N	2.43	0.42
1:D:137:GLN:O	1:D:141:GLU:HG3	2.20	0.42
1:D:146:ARG:HD3	1:D:149:ARG:NH2	2.33	0.42
1:A:212:LEU:O	1:A:212:LEU:HD12	2.20	0.41
1:D:121:LYS:HD2	1:D:123:LEU:CD2	2.50	0.41
1:D:35:VAL:O	1:D:35:VAL:CG1	2.64	0.41
1:C:149:ARG:HA	1:C:150:PRO:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:MET:O	1:C:20:GLN:HB2	2.21	0.41
1:D:220:ARG:CG	1:D:221:ASP:OD1	2.67	0.41
1:D:50:GLU:HA	1:D:53:LEU:HD12	2.02	0.41
1:A:96:GLU:OE2	1:A:97:GLY:HA2	2.20	0.41
1:B:49:LEU:CD1	1:B:146:ARG:NH2	2.83	0.41
1:C:44:GLY:N	1:C:155:GLU:OE1	2.38	0.41
1:C:156:LEU:HD13	1:C:175:TYR:HD2	1.85	0.41
1:B:184:LYS:C	1:B:186:ASP:N	2.52	0.41
1:C:165:ALA:O	1:C:169:LEU:HG	2.21	0.41
1:C:209:ASN:H	1:C:209:ASN:ND2	2.17	0.41
1:A:195:ILE:O	1:A:196:ASP:C	2.59	0.41
1:B:14:LYS:N	2:B:301:POP:O5	2.46	0.41
1:B:71:LEU:HD21	1:B:76:ALA:HA	2.02	0.41
1:D:195:ILE:HG23	1:D:200:HIS:HD2	1.82	0.41
1:A:162:TYR:CD2	1:A:162:TYR:N	2.89	0.41
1:A:28:PRO:HG2	1:A:93:LEU:HD22	2.01	0.41
1:C:191:GLN:C	1:C:193:PRO:HD2	2.41	0.41
1:D:128:SER:O	1:D:129:ASP:C	2.57	0.41
1:A:172:ILE:O	1:A:173:ASP:O	2.37	0.41
1:C:109:SER:HA	1:C:110:PRO:HD3	1.64	0.41
1:C:62:ASP:HB2	1:C:79:ARG:NH1	2.35	0.41
1:D:182:ALA:HA	1:D:187:LEU:HD12	2.02	0.41
1:B:40:GLN:HE21	1:B:40:GLN:HB3	1.58	0.41
1:C:185:HIS:O	1:C:186:ASP:HB3	2.21	0.41
1:D:64:ARG:HH11	1:D:64:ARG:HD2	1.58	0.41
1:A:179:ILE:O	1:A:182:ALA:N	2.54	0.41
1:A:217:SER:O	1:A:218:GLN:C	2.57	0.41
1:A:64:ARG:HA	1:A:65:PRO:HD3	1.89	0.41
1:B:210:GLU:HG3	1:B:210:GLU:O	2.21	0.41
1:C:165:ALA:O	1:C:169:LEU:N	2.34	0.41
1:B:131:PHE:HA	1:B:134:ARG:NH1	2.35	0.41
1:B:191:GLN:CA	1:B:191:GLN:HE21	2.33	0.41
1:B:34:ARG:NH1	1:B:73:ALA:N	2.69	0.41
1:C:137:GLN:O	1:C:141:GLU:HG3	2.21	0.41
1:C:40:GLN:HE21	1:C:40:GLN:HB3	1.48	0.41
1:C:5:LEU:HD12	1:C:95:LEU:O	2.21	0.41
1:D:43:THR:OG1	1:D:149:ARG:CD	2.68	0.41
1:D:3:LEU:HA	1:D:3:LEU:HD23	1.74	0.41
1:B:196:ASP:OD2	1:B:196:ASP:N	2.54	0.41
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.66	0.41
1:C:212:LEU:HB3	1:C:213:GLU:H	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:LEU:CD2	1:D:189:ILE:CG2	2.99	0.41
1:D:35:VAL:HG12	1:D:45:SER:HB2	2.02	0.41
1:A:120:VAL:HG21	1:A:225:TRP:HD1	1.86	0.40
1:A:13:GLY:O	1:A:17:MET:HG3	2.21	0.40
1:A:14:LYS:O	1:A:17:MET:N	2.54	0.40
1:A:173:ASP:HA	1:A:176:ARG:NH2	2.36	0.40
1:A:218:GLN:HB3	1:A:222:PHE:CE1	2.56	0.40
1:B:199:ARG:HA	1:B:202:GLU:OE2	2.22	0.40
1:B:20:GLN:HE21	1:B:20:GLN:HB3	1.79	0.40
1:D:64:ARG:HA	1:D:65:PRO:HD3	1.82	0.40
1:C:174:GLY:HA2	1:C:207:ILE:HG12	2.04	0.40
1:C:209:ASN:ND2	1:C:209:ASN:N	2.69	0.40
1:D:195:ILE:CG2	1:D:200:HIS:CD2	2.97	0.40
1:D:124:ARG:HD2	1:D:219:GLU:OE1	2.21	0.40
1:A:131:PHE:CD1	1:A:212:LEU:CD1	2.94	0.40
1:A:207:ILE:O	1:A:210:GLU:N	2.54	0.40
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.79	0.40
1:C:182:ALA:C	1:C:184:LYS:H	2.24	0.40
1:C:33:ASP:CG	1:C:36:GLN:HB2	2.42	0.40
1:D:144:ALA:HB3	1:D:149:ARG:NH2	2.37	0.40
1:D:25:THR:CG2	1:D:27:TRP:CG	3.02	0.40
1:A:192:LEU:N	1:A:193:PRO:HD2	2.37	0.40
1:A:3:LEU:HA	1:A:3:LEU:HD23	1.55	0.40
1:A:94:ILE:H	1:A:94:ILE:HG13	1.66	0.40
1:B:14:LYS:O	1:B:15:THR:C	2.60	0.40
1:A:14:LYS:O	1:A:15:THR:C	2.59	0.40
1:A:176:ARG:NH1	1:A:210:GLU:OE1	2.55	0.40
1:A:34:ARG:HH12	1:A:72:ASP:HA	1.87	0.40
1:A:64:ARG:HD2	1:A:64:ARG:HH11	1.53	0.40
1:C:81:ILE:HG12	1:C:111:PHE:CD2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLU:OE1	1:B:185:HIS:ND1[4_545]	2.11	0.09

## 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	224/253 (88%)	185 (83%)	31 (14%)	8 (4%)	3	11
1	B	224/253 (88%)	180 (80%)	30 (13%)	14 (6%)	1	3
1	C	224/253 (88%)	183 (82%)	32 (14%)	9 (4%)	3	9
1	D	224/253 (88%)	191 (85%)	21 (9%)	12 (5%)	2	5
All	All	896/1012 (88%)	739 (82%)	114 (13%)	43 (5%)	2	7

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	SER
1	A	150	PRO
1	A	174	GLY
1	A	196	ASP
1	B	42	ALA
1	B	114	SER
1	B	173	ASP
1	B	185	HIS
1	B	190	SER
1	C	114	SER
1	C	150	PRO
1	C	197	ALA
1	D	42	ALA
1	D	114	SER
1	D	157	ALA
1	D	196	ASP
1	A	173	ASP
1	B	76	ALA
1	B	174	GLY
1	B	184	LYS
1	B	204	ILE
1	C	196	ASP

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Mol	Chain	Res	Type
1	D	197	ALA
1	D	208	ALA
1	A	170	GLU
1	D	198	GLY
1	B	196	ASP
1	C	36	GLN
1	C	191	GLN
1	A	42	ALA
1	A	157	ALA
1	B	170	GLU
1	B	205	GLU
1	D	158	GLU
1	D	170	GLU
1	C	42	ALA
1	C	190	SER
1	D	179	ILE
1	D	180	ARG
1	B	193	PRO
1	D	223	PRO
1	C	174	GLY
1	B	223	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/215 (89%)	144 (75%)	48 (25%)	0	2
1	B	192/215 (89%)	143 (74%)	49 (26%)	0	1
1	C	192/215 (89%)	144 (75%)	48 (25%)	0	2
1	D	192/215 (89%)	146 (76%)	46 (24%)	0	2
All	All	768/860 (89%)	577 (75%)	191 (25%)	0	2

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	12	SER
1	A	20	GLN
1	A	23	GLN
1	A	25	THR
1	A	34	ARG
1	A	40	GLN
1	A	62	ASP
1	A	63	SER
1	A	65	PRO
1	A	66	LEU
1	A	68	GLU
1	A	70	ILE
1	A	72	ASP
1	A	74	GLU
1	A	78	ARG
1	A	88	LYS
1	A	96	GLU
1	A	100	ILE
1	A	103	LEU
1	A	108	LYS
1	A	114	SER
1	A	116	PHE
1	A	117	GLN
1	A	119	HIS
1	A	124	ARG
1	A	127	ASP
1	A	132	LEU
1	A	148	ASP
1	A	149	ARG
1	A	159	LEU
1	A	161	ASN
1	A	168	ILE
1	A	171	ASP
1	A	181	PHE
1	A	183	ARG
1	A	184	LYS
1	A	187	LEU
1	A	189	ILE
1	A	190	SER
1	A	191	GLN
1	A	194	ASN
1	A	195	ILE

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Mol	Chain	Res	Type
1	A	202	GLU
1	A	209	ASN
1	A	216	LEU
1	A	220	ARG
1	A	224	GLN
1	B	2	LEU
1	B	12	SER
1	B	20	GLN
1	B	25	THR
1	B	34	ARG
1	B	36	GLN
1	B	37	CYS
1	B	40	GLN
1	B	41	ILE
1	B	47	ARG
1	B	62	ASP
1	B	66	LEU
1	B	68	GLU
1	B	72	ASP
1	B	74	GLU
1	B	78	ARG
1	B	88	LYS
1	B	96	GLU
1	B	100	ILE
1	B	103	LEU
1	B	108	LYS
1	B	114	SER
1	B	116	PHE
1	B	117	GLN
1	B	119	HIS
1	B	124	ARG
1	B	127	ASP
1	B	132	LEU
1	B	148	ASP
1	B	149	ARG
1	B	151	SER
1	B	159	LEU
1	B	161	ASN
1	B	169	LEU
1	B	171	ASP
1	B	176	ARG
1	B	183	ARG

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Mol	Chain	Res	Type
1	B	184	LYS
1	B	191	GLN
1	B	194	ASN
1	B	195	ILE
1	B	200	HIS
1	B	201	VAL
1	B	209	ASN
1	B	210	GLU
1	B	219	GLU
1	B	220	ARG
1	B	224	GLN
1	B	225	TRP
1	C	2	LEU
1	C	12	SER
1	C	20	GLN
1	C	23	GLN
1	C	25	THR
1	C	34	ARG
1	C	37	CYS
1	C	40	GLN
1	C	41	ILE
1	C	47	ARG
1	C	62	ASP
1	C	63	SER
1	C	66	LEU
1	C	70	ILE
1	C	74	GLU
1	C	75	SER
1	C	78	ARG
1	C	88	LYS
1	C	96	GLU
1	C	100	ILE
1	C	103	LEU
1	C	108	LYS
1	C	114	SER
1	C	116	PHE
1	C	117	GLN
1	C	119	HIS
1	C	124	ARG
1	C	127	ASP
1	C	132	LEU
1	C	148	ASP

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Mol	Chain	Res	Type
1	C	149	ARG
1	C	156	LEU
1	C	168	ILE
1	C	171	ASP
1	C	172	ILE
1	C	176	ARG
1	C	183	ARG
1	C	184	LYS
1	C	187	LEU
1	C	190	SER
1	C	191	GLN
1	C	194	ASN
1	C	195	ILE
1	C	200	HIS
1	C	202	GLU
1	C	213	GLU
1	C	216	LEU
1	C	224	GLN
1	D	2	LEU
1	D	12	SER
1	D	20	GLN
1	D	23	GLN
1	D	25	THR
1	D	34	ARG
1	D	40	GLN
1	D	47	ARG
1	D	62	ASP
1	D	63	SER
1	D	65	PRO
1	D	66	LEU
1	D	68	GLU
1	D	72	ASP
1	D	74	GLU
1	D	78	ARG
1	D	88	LYS
1	D	96	GLU
1	D	100	ILE
1	D	103	LEU
1	D	108	LYS
1	D	114	SER
1	D	116	PHE
1	D	117	GLN

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Mol	Chain	Res	Type
1	D	119	HIS
1	D	124	ARG
1	D	127	ASP
1	D	132	LEU
1	D	148	ASP
1	D	149	ARG
1	D	159	LEU
1	D	161	ASN
1	D	168	ILE
1	D	170	GLU
1	D	171	ASP
1	D	181	PHE
1	D	183	ARG
1	D	184	LYS
1	D	187	LEU
1	D	195	ILE
1	D	200	HIS
1	D	202	GLU
1	D	209	ASN
1	D	213	GLU
1	D	220	ARG
1	D	224	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	20	GLN
1	A	23	GLN
1	A	40	GLN
1	A	161	ASN
1	A	200	HIS
1	A	209	ASN
1	A	224	GLN
1	B	4	HIS
1	B	20	GLN
1	B	23	GLN
1	B	40	GLN
1	B	161	ASN
1	B	191	GLN
1	B	200	HIS
1	B	209	ASN

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Mol	Chain	Res	Type
1	B	224	GLN
1	C	4	HIS
1	C	20	GLN
1	C	23	GLN
1	C	40	GLN
1	C	191	GLN
1	C	200	HIS
1	C	209	ASN
1	C	214	HIS
1	C	224	GLN
1	D	4	HIS
1	D	20	GLN
1	D	23	GLN
1	D	40	GLN
1	D	54	GLN
1	D	161	ASN
1	D	191	GLN
1	D	200	HIS
1	D	209	ASN
1	D	224	GLN

### 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](#)

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	POP	A	301	-	6,8,8	1.10	0	13,13,13	1.51	2 (15%)
2	POP	C	301	-	6,8,8	1.60	2 (33%)	13,13,13	2.18	4 (30%)
2	POP	B	301	-	6,8,8	1.59	1 (16%)	13,13,13	1.44	2 (15%)
2	POP	D	301	-	6,8,8	1.53	1 (16%)	13,13,13	2.10	6 (46%)

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	POP	A	301	-	-	0/6/6/6	-
2	POP	C	301	-	-	0/6/6/6	-
2	POP	B	301	-	-	1/6/6/6	-
2	POP	D	301	-	-	5/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	POP	P1-O1	3.10	1.60	1.50
2	D	301	POP	P1-O1	2.95	1.60	1.50
2	C	301	POP	P1-O1	2.27	1.57	1.50
2	C	301	POP	P2-O6	-2.03	1.47	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	POP	O2-P1-O	5.00	121.41	104.64
2	C	301	POP	O3-P1-O2	4.15	123.49	107.64
2	D	301	POP	O6-P2-O	3.77	117.29	104.64
2	D	301	POP	O3-P1-O	3.65	116.87	104.64
2	B	301	POP	O6-P2-O	3.53	116.47	104.64
2	A	301	POP	O3-P1-O2	2.67	117.84	107.64
2	D	301	POP	O6-P2-O5	2.63	117.70	107.64
2	B	301	POP	O3-P1-O2	2.44	116.95	107.64
2	D	301	POP	O5-P2-O	-2.34	96.78	104.64
2	C	301	POP	O2-P1-O1	-2.25	101.87	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	POP	O2-P1-O	-2.07	97.68	104.64
2	C	301	POP	O-P1-O1	-2.05	99.81	111.19
2	A	301	POP	O6-P2-O5	2.05	115.46	107.64
2	D	301	POP	O2-P1-O1	2.02	118.57	110.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	POP	P2-O-P1-O3
2	D	301	POP	P1-O-P2-O6
2	B	301	POP	P1-O-P2-O5
2	D	301	POP	P1-O-P2-O5
2	D	301	POP	P1-O-P2-O4
2	D	301	POP	P2-O-P1-O1

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	POP	1	0
2	B	301	POP	2	0
2	D	301	POP	1	0

## 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, 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	226/253 (89%)	0.31	7 (3%) 49 39	65, 85, 105, 112	0
1	B	226/253 (89%)	0.26	9 (3%) 38 28	65, 85, 104, 111	0
1	C	226/253 (89%)	0.24	8 (3%) 44 34	65, 85, 105, 111	0
1	D	226/253 (89%)	0.16	8 (3%) 44 34	65, 85, 104, 112	0
All	All	904/1012 (89%)	0.24	32 (3%) 44 34	65, 85, 105, 112	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	GLY	5.2
1	C	95	LEU	4.1
1	A	108	LYS	3.9
1	D	112	TRP	3.8
1	A	3	LEU	3.7
1	B	160	TRP	3.6
1	D	116	PHE	3.5
1	D	211	TYR	2.8
1	A	114	SER	2.8
1	A	221	ASP	2.7
1	B	120	VAL	2.6
1	C	114	SER	2.6
1	D	95	LEU	2.5
1	A	197	ALA	2.4
1	B	180	ARG	2.4
1	C	225	TRP	2.4
1	C	5	LEU	2.4
1	D	84	VAL	2.4
1	B	106	MET	2.4
1	B	189	ILE	2.3
1	C	132	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	118	TRP	2.3
1	D	115	GLY	2.3
1	B	25	THR	2.3
1	D	203	LEU	2.3
1	B	133	THR	2.3
1	C	30	VAL	2.2
1	C	10	THR	2.2
1	D	225	TRP	2.1
1	B	216	LEU	2.1
1	B	197	ALA	2.1
1	C	156	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	POP	C	301	9/9	0.92	0.12	92,94,98,99	0
2	POP	B	301	9/9	0.93	0.10	89,89,92,92	0
2	POP	D	301	9/9	0.95	0.12	83,86,87,88	0
2	POP	A	301	9/9	0.96	0.11	89,90,91,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.