



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:11 PM UTC

PDB ID : 2ZE8 / pdb_00002ze8
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

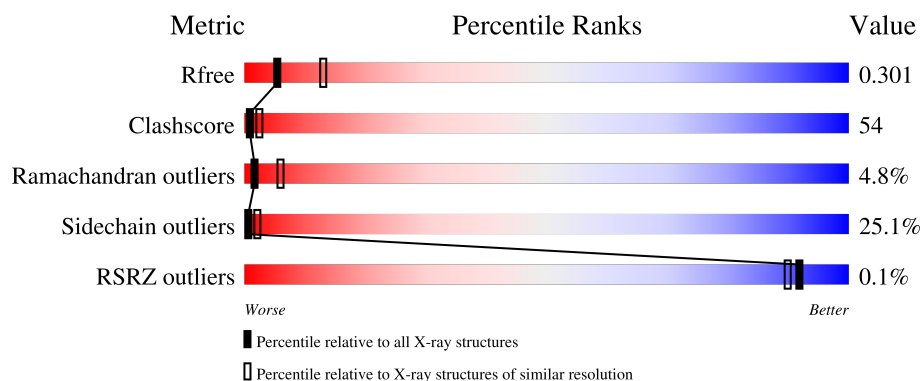
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	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 criteria:

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:

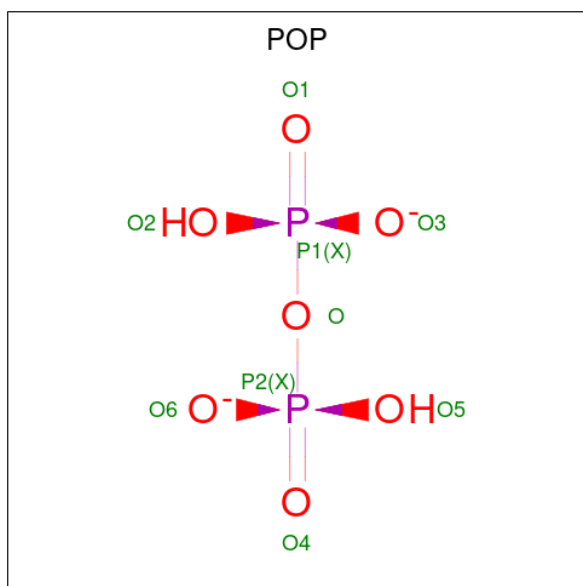
Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	expression tag	UNP P58758
A	245	SER	-	expression tag	UNP P58758
A	246	ARG	-	expression tag	UNP P58758
A	247	SER	-	expression tag	UNP P58758
A	248	HIS	-	expression tag	UNP P58758
A	249	HIS	-	expression tag	UNP P58758
A	250	HIS	-	expression tag	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- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).

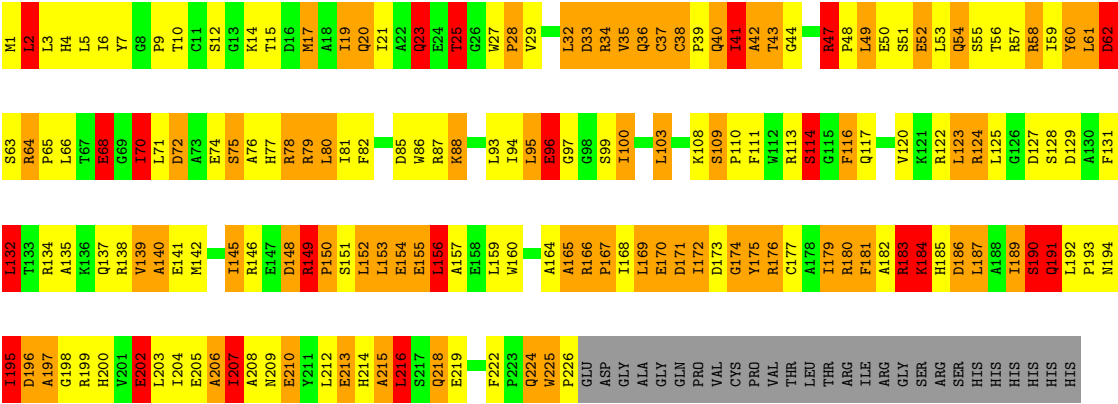


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			9	7	2		
2	B	1	Total	O	P	0	0
			9	7	2		

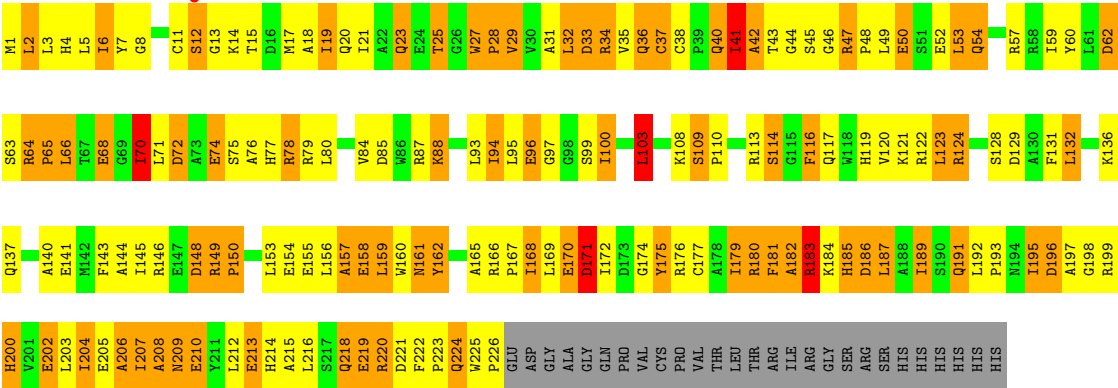
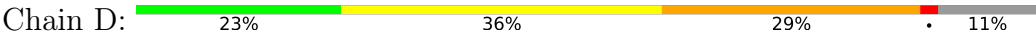
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	P	0	0
			9	7	2		
2	D	1	Total	O	P	0	0
			9	7	2		



• Molecule 1: Isopentenyl transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.51Å 97.57Å 131.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	131.31 – 2.80 131.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (131.31-2.80) 97.7 (131.11-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 79.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.88	40/1856 (2.2%)	1.93	60/2514 (2.4%)
1	B	1.91	43/1856 (2.3%)	1.84	52/2514 (2.1%)
1	C	2.08	63/1856 (3.4%)	2.08	59/2514 (2.3%)
1	D	1.65	19/1856 (1.0%)	1.76	52/2514 (2.1%)
All	All	1.89	165/7424 (2.2%)	1.91	223/10056 (2.2%)

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 (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	ASP	CG-OD1	13.58	1.51	1.25
1	C	186	ASP	CG-OD2	11.46	1.47	1.25
1	C	60	TYR	N-CA	11.39	1.59	1.46
1	B	60	TYR	CA-C	10.92	1.66	1.52
1	A	59	ILE	CA-CB	-10.89	1.41	1.54
1	C	183	ARG	CZ-NH1	10.28	1.47	1.32
1	A	207	ILE	CA-CB	-8.98	1.42	1.54
1	C	207	ILE	CA-CB	-8.94	1.42	1.54
1	C	175	TYR	CA-C	8.89	1.64	1.52
1	C	94	ILE	CA-CB	-8.80	1.43	1.54
1	B	70	ILE	CA-CB	-8.68	1.44	1.54
1	B	94	ILE	CA-CB	-8.58	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	ILE	CA-CB	-8.37	1.43	1.54
1	C	172	ILE	CA-CB	-8.37	1.43	1.54
1	C	184	LYS	CE-NZ	8.27	1.74	1.49
1	D	70	ILE	CA-CB	-8.17	1.45	1.54
1	C	38	CYS	CA-CB	-8.07	1.42	1.53
1	B	60	TYR	N-CA	7.75	1.56	1.46
1	C	70	ILE	CA-CB	-7.73	1.44	1.54
1	C	58	ARG	CA-C	7.72	1.62	1.52
1	B	179	ILE	CA-CB	-7.69	1.43	1.54
1	D	207	ILE	CA-CB	-7.66	1.46	1.54
1	C	183	ARG	CZ-NH2	7.66	1.43	1.33
1	C	58	ARG	C-O	7.66	1.32	1.24
1	C	164	ALA	CA-C	7.60	1.63	1.52
1	B	70	ILE	C-O	7.50	1.33	1.24
1	A	59	ILE	N-CA	7.48	1.55	1.46
1	D	59	ILE	CA-CB	-7.47	1.45	1.54
1	C	29	VAL	CA-CB	-7.35	1.45	1.54
1	A	176	ARG	CA-C	-7.30	1.43	1.52
1	C	152	LEU	N-CA	-7.27	1.36	1.46
1	B	61	LEU	N-CA	7.26	1.55	1.46
1	B	53	LEU	C-O	7.13	1.33	1.24
1	C	79	ARG	C-O	-7.13	1.15	1.24
1	A	18	ALA	CA-CB	-7.12	1.42	1.53
1	C	139	VAL	CA-CB	-7.02	1.45	1.54
1	C	80	LEU	C-O	7.00	1.32	1.24
1	C	42	ALA	CA-CB	-6.99	1.41	1.53
1	A	95	LEU	CA-C	-6.97	1.44	1.52
1	B	207	ILE	CA-CB	-6.97	1.46	1.54
1	B	81	ILE	CA-CB	-6.96	1.46	1.54
1	A	57	ARG	CA-C	6.94	1.61	1.52
1	B	18	ALA	CA-CB	-6.94	1.42	1.53
1	D	41	ILE	CA-CB	-6.94	1.45	1.54
1	D	18	ALA	CA-CB	-6.93	1.42	1.53
1	C	60	TYR	CZ-OH	6.83	1.52	1.38
1	C	62	ASP	C-O	-6.81	1.17	1.24
1	B	61	LEU	C-O	-6.77	1.15	1.24
1	A	64	ARG	CA-CB	-6.68	1.44	1.53
1	A	41	ILE	CA-CB	-6.68	1.45	1.54
1	B	177	CYS	N-CA	-6.67	1.38	1.46
1	B	30	VAL	C-O	6.65	1.32	1.24
1	A	53	LEU	N-CA	-6.62	1.37	1.46
1	B	78	ARG	CA-C	6.57	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	155	GLU	CA-C	-6.57	1.43	1.52
1	A	61	LEU	C-O	6.54	1.32	1.24
1	A	70	ILE	C-O	-6.54	1.15	1.24
1	B	152	LEU	C-O	6.47	1.31	1.24
1	C	96	GLU	CA-C	-6.46	1.44	1.52
1	B	39	PRO	C-O	-6.45	1.16	1.24
1	A	85	ASP	C-O	-6.41	1.16	1.24
1	C	183	ARG	CD-NE	6.38	1.55	1.46
1	A	37	CYS	CA-CB	-6.36	1.43	1.53
1	A	152	LEU	C-O	-6.33	1.16	1.24
1	A	94	ILE	CA-CB	-6.31	1.46	1.54
1	A	103	LEU	CA-C	-6.30	1.44	1.52
1	D	175	TYR	C-O	-6.29	1.16	1.24
1	A	42	ALA	CA-CB	-6.29	1.42	1.53
1	B	149	ARG	C-O	6.27	1.31	1.24
1	C	169	LEU	CA-C	6.23	1.61	1.52
1	B	96	GLU	CA-C	-6.12	1.45	1.52
1	D	94	ILE	CA-CB	-6.10	1.46	1.54
1	C	38	CYS	N-CA	-6.09	1.40	1.46
1	B	27	TRP	C-O	6.07	1.31	1.23
1	B	175	TYR	N-CA	-6.02	1.38	1.46
1	B	52	GLU	CA-C	-5.99	1.44	1.52
1	C	170	GLU	N-CA	-5.97	1.37	1.46
1	A	55	SER	CA-C	5.95	1.60	1.52
1	A	47	ARG	C-O	-5.92	1.16	1.24
1	C	94	ILE	N-CA	-5.92	1.39	1.46
1	B	186	ASP	CA-C	-5.91	1.45	1.53
1	B	59	ILE	CB-CG2	5.91	1.72	1.52
1	A	7	TYR	CA-C	-5.88	1.45	1.52
1	D	28	PRO	N-CA	-5.81	1.40	1.47
1	B	60	TYR	CB-CG	-5.78	1.39	1.51
1	B	92	GLY	C-O	-5.77	1.17	1.23
1	B	217	SER	C-N	5.74	1.41	1.34
1	D	219	GLU	N-CA	-5.71	1.39	1.46
1	C	171	ASP	CA-C	5.66	1.60	1.52
1	C	149	ARG	CG-CD	5.63	1.69	1.52
1	A	47	ARG	CA-C	-5.61	1.47	1.53
1	C	157	ALA	N-CA	5.60	1.53	1.46
1	A	122	ARG	C-O	-5.60	1.17	1.24
1	A	102	LEU	CA-C	5.60	1.60	1.52
1	A	94	ILE	CA-C	5.58	1.59	1.52
1	C	72	ASP	C-O	-5.54	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	175	TYR	CD1-CE1	5.54	1.55	1.38
1	B	59	ILE	CA-CB	-5.54	1.47	1.54
1	A	180	ARG	CZ-NH1	5.52	1.40	1.32
1	A	70	ILE	CA-CB	-5.51	1.47	1.54
1	A	52	GLU	N-CA	5.51	1.54	1.46
1	C	206	ALA	CA-CB	-5.50	1.44	1.53
1	C	64	ARG	N-CA	5.48	1.51	1.45
1	C	41	ILE	CA-C	-5.47	1.45	1.52
1	A	169	LEU	N-CA	5.47	1.52	1.46
1	D	53	LEU	CA-C	-5.43	1.45	1.52
1	A	130	ALA	CA-CB	-5.42	1.44	1.53
1	C	172	ILE	N-CA	-5.41	1.40	1.46
1	A	87	ARG	N-CA	-5.40	1.39	1.46
1	C	47	ARG	CA-CB	5.40	1.61	1.53
1	C	59	ILE	CA-CB	-5.39	1.47	1.54
1	D	182	ALA	N-CA	5.38	1.52	1.46
1	A	184	LYS	C-O	-5.37	1.18	1.24
1	B	224	GLN	N-CA	5.36	1.52	1.45
1	D	28	PRO	CA-CB	-5.34	1.46	1.53
1	B	76	ALA	C-O	5.33	1.30	1.24
1	C	49	LEU	CA-C	-5.33	1.45	1.53
1	C	184	LYS	C-O	-5.33	1.17	1.23
1	B	27	TRP	CA-C	5.32	1.59	1.53
1	C	181	PHE	CA-C	5.32	1.59	1.52
1	D	150	PRO	C-O	-5.31	1.17	1.23
1	C	23	GLN	N-CA	-5.31	1.40	1.46
1	C	61	LEU	N-CA	5.31	1.52	1.46
1	A	41	ILE	CB-CG2	-5.29	1.35	1.52
1	A	71	LEU	N-CA	-5.27	1.39	1.46
1	C	165	ALA	CA-CB	-5.27	1.44	1.53
1	B	30	VAL	CA-CB	-5.26	1.48	1.54
1	B	41	ILE	CA-CB	-5.26	1.47	1.54
1	C	25	THR	CA-C	5.26	1.59	1.52
1	C	17	MET	CA-C	-5.22	1.46	1.52
1	C	57	ARG	CA-C	5.22	1.59	1.52
1	B	60	TYR	CZ-OH	5.21	1.49	1.38
1	B	177	CYS	CB-SG	-5.21	1.64	1.81
1	D	64	ARG	CA-CB	-5.21	1.46	1.54
1	A	57	ARG	NE-CZ	5.20	1.38	1.33
1	B	165	ALA	CA-CB	-5.17	1.44	1.53
1	C	145	ILE	CA-CB	-5.16	1.48	1.54
1	B	64	ARG	CG-CD	-5.15	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	95	LEU	CA-C	-5.15	1.46	1.52
1	B	50	GLU	CD-OE2	5.14	1.35	1.25
1	B	48	PRO	CA-C	-5.13	1.46	1.52
1	C	222	PHE	CA-C	-5.12	1.46	1.53
1	D	189	ILE	N-CA	-5.12	1.40	1.46
1	C	86	TRP	C-O	-5.12	1.16	1.24
1	C	149	ARG	CD-NE	5.10	1.53	1.46
1	D	175	TYR	CA-C	-5.10	1.46	1.52
1	A	66	LEU	CA-C	5.10	1.60	1.52
1	C	213	GLU	N-CA	-5.09	1.40	1.46
1	B	55	SER	N-CA	5.09	1.52	1.46
1	B	213	GLU	CA-C	-5.09	1.46	1.52
1	A	81	ILE	CA-C	-5.09	1.46	1.52
1	C	28	PRO	N-CA	5.08	1.53	1.47
1	D	171	ASP	C-O	-5.08	1.17	1.24
1	C	149	ARG	CZ-NH1	5.08	1.39	1.32
1	B	220	ARG	CZ-NH1	5.07	1.39	1.32
1	C	180	ARG	CG-CD	5.06	1.67	1.52
1	C	48	PRO	CA-C	-5.04	1.46	1.52
1	D	103	LEU	CA-C	-5.03	1.45	1.52
1	A	71	LEU	CA-C	-5.03	1.46	1.52
1	A	178	ALA	CA-CB	-5.02	1.45	1.53
1	C	180	ARG	CZ-NH1	5.01	1.39	1.32
1	B	41	ILE	C-O	5.01	1.30	1.24
1	C	43	THR	C-O	5.01	1.29	1.24
1	D	63	SER	C-O	-5.01	1.18	1.24
1	C	33	ASP	N-CA	-5.01	1.40	1.46

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	GLU	N-CA-C	-19.02	88.27	112.23
1	C	222	PHE	CA-C-N	-16.15	99.65	119.84
1	C	222	PHE	C-N-CA	-16.15	99.65	119.84
1	C	152	LEU	N-CA-C	-13.77	96.16	113.23
1	A	155	GLU	N-CA-C	-13.30	96.77	111.14
1	C	179	ILE	N-CA-C	10.41	120.31	110.53
1	A	222	PHE	CA-C-N	-9.95	107.40	119.84
1	A	222	PHE	C-N-CA	-9.95	107.40	119.84
1	C	109	SER	CA-C-N	9.93	130.07	119.05
1	C	109	SER	C-N-CA	9.93	130.07	119.05
1	A	29	VAL	CB-CA-C	-9.79	97.60	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	ILE	N-CA-C	9.64	119.68	110.42
1	B	78	ARG	N-CA-C	-9.47	100.64	110.97
1	B	109	SER	CA-C-N	9.26	128.94	118.85
1	B	109	SER	C-N-CA	9.26	128.94	118.85
1	D	186	ASP	CA-C-N	-9.00	105.46	122.73
1	D	186	ASP	C-N-CA	-9.00	105.46	122.73
1	C	218	GLN	N-CA-C	-8.91	101.52	111.14
1	C	47	ARG	N-CA-C	-8.88	97.83	110.08
1	A	109	SER	CA-C-N	8.85	129.02	119.28
1	A	109	SER	C-N-CA	8.85	129.02	119.28
1	C	167	PRO	N-CA-C	-8.85	100.81	113.47
1	B	78	ARG	CB-CA-C	8.69	124.34	110.96
1	C	10	THR	CA-C-N	-8.63	109.32	123.04
1	C	10	THR	C-N-CA	-8.63	109.32	123.04
1	A	64	ARG	CA-C-N	8.52	129.03	119.83
1	A	64	ARG	C-N-CA	8.52	129.03	119.83
1	A	176	ARG	N-CA-C	-8.48	100.94	111.11
1	C	47	ARG	CA-C-N	8.43	128.57	120.31
1	C	47	ARG	C-N-CA	8.43	128.57	120.31
1	B	183	ARG	N-CA-C	-8.41	103.00	113.18
1	B	64	ARG	N-CA-C	8.37	118.91	108.11
1	D	64	ARG	CA-C-N	8.19	128.68	119.83
1	D	64	ARG	C-N-CA	8.19	128.68	119.83
1	A	47	ARG	N-CA-C	-8.10	99.54	109.83
1	B	64	ARG	CA-C-N	8.03	128.52	119.93
1	B	64	ARG	C-N-CA	8.03	128.52	119.93
1	B	154	GLU	N-CA-C	-7.89	102.62	111.14
1	C	154	GLU	N-CA-C	-7.88	103.79	113.41
1	A	191	GLN	N-CA-C	-7.87	105.65	114.62
1	D	50	GLU	N-CA-C	-7.86	102.02	111.69
1	D	29	VAL	CB-CA-C	-7.84	99.51	110.96
1	B	73	ALA	N-CA-C	7.82	119.43	111.07
1	A	80	LEU	CA-C-O	7.79	129.64	121.07
1	C	215	ALA	N-CA-C	-7.77	102.78	111.71
1	C	172	ILE	CB-CA-C	-7.75	100.14	111.68
1	D	78	ARG	N-CA-C	-7.71	102.82	111.14
1	B	52	GLU	N-CA-CB	7.70	122.22	110.44
1	B	60	TYR	N-CA-C	7.70	122.90	109.96
1	A	210	GLU	N-CA-C	-7.70	102.48	111.03
1	B	29	VAL	CB-CA-C	-7.65	100.56	111.19
1	D	109	SER	CA-C-N	7.64	127.68	119.28
1	D	109	SER	C-N-CA	7.64	127.68	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	GLN	N-CA-C	-7.56	103.02	111.71
1	D	210	GLU	N-CA-C	-7.56	103.12	111.36
1	D	150	PRO	N-CA-C	-7.42	100.72	111.33
1	C	64	ARG	N-CA-C	7.41	116.85	108.25
1	C	29	VAL	CB-CA-C	-7.39	100.17	110.96
1	B	50	GLU	N-CA-C	-7.39	103.31	111.36
1	D	140	ALA	N-CA-C	-7.34	103.28	111.28
1	C	47	ARG	CA-CB-CG	7.27	128.64	114.10
1	A	218	GLN	N-CA-C	-7.19	102.48	111.11
1	A	68	GLU	N-CA-C	-7.18	104.40	113.02
1	B	27	TRP	N-CA-C	7.08	119.85	110.08
1	D	64	ARG	N-CA-C	7.06	114.58	108.22
1	D	78	ARG	CB-CA-C	7.04	122.02	110.90
1	C	159	LEU	N-CA-C	-7.03	104.58	113.01
1	C	153	LEU	N-CA-C	-7.02	104.69	113.18
1	C	78	ARG	CB-CA-C	7.00	121.73	110.96
1	B	52	GLU	N-CA-C	-6.90	104.60	113.16
1	B	64	ARG	NE-CZ-NH1	-6.88	114.62	121.50
1	D	162	TYR	CA-C-N	-6.85	111.39	118.85
1	D	162	TYR	C-N-CA	-6.85	111.39	118.85
1	A	71	LEU	N-CA-C	-6.81	99.75	109.96
1	B	68	GLU	N-CA-C	-6.81	105.05	113.15
1	B	43	THR	CB-CA-C	-6.80	100.21	110.88
1	B	105	CYS	CA-CB-SG	-6.78	98.81	114.40
1	C	156	LEU	N-CA-C	6.71	118.25	111.07
1	C	54	GLN	CB-CA-C	-6.66	102.27	111.73
1	D	6	ILE	CB-CA-C	-6.60	101.51	110.42
1	A	175	TYR	CA-C-N	6.55	129.39	120.54
1	A	175	TYR	C-N-CA	6.55	129.39	120.54
1	D	64	ARG	N-CA-CB	-6.54	104.23	111.10
1	B	47	ARG	CA-CB-CG	6.54	127.17	114.10
1	C	68	GLU	N-CA-C	-6.53	105.38	113.15
1	C	225	TRP	N-CA-C	6.46	118.22	109.24
1	A	33	ASP	CB-CA-C	-6.46	102.96	111.42
1	A	140	ALA	N-CA-C	-6.42	103.56	111.33
1	A	64	ARG	NE-CZ-NH1	-6.39	115.11	121.50
1	D	12	SER	N-CA-C	-6.38	103.95	112.94
1	A	10	THR	CA-C-N	-6.37	111.78	122.92
1	A	10	THR	C-N-CA	-6.37	111.78	122.92
1	C	52	GLU	N-CA-CB	6.36	120.18	110.44
1	A	47	ARG	CA-CB-CG	6.33	126.75	114.10
1	B	35	VAL	CB-CA-C	-6.30	102.06	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	ILE	N-CA-CB	6.30	117.92	110.55
1	D	37	CYS	N-CA-C	-6.24	105.42	113.16
1	B	166	ARG	N-CA-C	6.21	120.67	112.35
1	A	93	LEU	CB-CG-CD1	-6.20	92.11	110.70
1	B	224	GLN	N-CA-C	6.19	120.13	110.17
1	C	210	GLU	N-CA-C	-6.17	104.56	111.28
1	B	32	LEU	CA-CB-CG	-6.15	94.79	116.30
1	B	104	ASN	N-CA-C	-6.12	104.72	111.82
1	C	70	ILE	N-CA-C	-6.11	100.89	109.21
1	C	96	GLU	N-CA-C	-6.11	98.31	108.75
1	D	68	GLU	N-CA-C	-6.10	106.10	112.93
1	A	94	ILE	N-CA-C	6.08	117.48	109.21
1	C	170	GLU	N-CA-C	-6.06	105.98	113.19
1	D	159	LEU	N-CA-C	6.05	119.49	111.75
1	D	214	HIS	N-CA-C	-6.04	104.60	111.07
1	A	2	LEU	N-CA-C	6.04	119.37	109.76
1	B	84	VAL	CA-C-N	-6.03	112.69	120.65
1	B	84	VAL	C-N-CA	-6.03	112.69	120.65
1	A	172	ILE	N-CA-CB	-6.01	102.02	110.26
1	A	17	MET	N-CA-C	-6.01	104.42	110.97
1	B	48	PRO	CB-CA-C	-5.99	103.11	110.95
1	A	77	HIS	N-CA-C	5.98	117.80	111.28
1	B	140	ALA	N-CA-C	-5.97	103.94	111.11
1	A	54	GLN	CB-CA-C	-5.96	103.52	111.63
1	C	47	ARG	CB-CA-C	-5.93	99.72	109.27
1	C	49	LEU	N-CA-C	-5.93	102.54	110.55
1	A	78	ARG	CB-CA-C	5.87	120.17	110.90
1	D	4	HIS	CA-C-N	-5.87	114.42	122.93
1	D	4	HIS	C-N-CA	-5.87	114.42	122.93
1	D	59	ILE	CB-CA-C	-5.86	102.71	110.98
1	B	87	ARG	N-CA-C	-5.84	105.34	112.88
1	D	32	LEU	CA-CB-CG	-5.83	95.89	116.30
1	D	218	GLN	CA-C-N	-5.82	112.87	120.44
1	D	218	GLN	C-N-CA	-5.82	112.87	120.44
1	A	4	HIS	CA-C-N	-5.82	114.50	122.93
1	A	4	HIS	C-N-CA	-5.82	114.50	122.93
1	B	168	ILE	N-CA-C	-5.79	104.86	110.42
1	C	2	LEU	N-CA-C	5.76	119.30	110.20
1	C	179	ILE	CB-CA-C	-5.75	104.49	112.02
1	A	29	VAL	N-CA-CB	-5.74	104.23	111.41
1	A	44	GLY	N-CA-C	-5.67	105.51	112.77
1	A	60	TYR	CA-C-O	5.67	126.72	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	LEU	CA-C-N	-5.64	112.28	120.29
1	A	132	LEU	C-N-CA	-5.64	112.28	120.29
1	D	54	GLN	CB-CA-C	-5.64	103.73	111.73
1	C	132	LEU	CA-C-N	-5.62	112.80	120.44
1	C	132	LEU	C-N-CA	-5.62	112.80	120.44
1	A	12	SER	N-CA-C	-5.61	105.64	112.88
1	C	166	ARG	CA-C-N	-5.61	113.14	118.97
1	C	166	ARG	C-N-CA	-5.61	113.14	118.97
1	C	47	ARG	CA-C-O	-5.59	114.61	120.70
1	A	204	ILE	N-CA-CB	5.58	116.71	110.62
1	D	204	ILE	CB-CA-C	-5.57	104.74	112.04
1	A	149	ARG	CG-CD-NE	5.56	124.24	112.00
1	A	23	GLN	CB-CG-CD	-5.56	103.14	112.60
1	B	64	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	A	103	LEU	N-CA-C	-5.55	106.64	113.41
1	A	57	ARG	N-CA-C	5.54	117.76	108.73
1	A	172	ILE	CA-C-O	-5.53	114.53	121.11
1	A	149	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	A	43	THR	CB-CA-C	-5.52	102.21	110.88
1	B	79	ARG	CA-C-O	-5.49	114.60	121.02
1	D	64	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	D	46	GLY	CA-C-O	-5.47	113.05	118.96
1	A	85	ASP	N-CA-C	5.47	117.69	111.02
1	D	183	ARG	N-CA-C	-5.45	105.73	112.38
1	B	171	ASP	N-CA-C	5.43	120.18	113.50
1	D	167	PRO	CA-C-N	-5.42	113.73	120.56
1	D	167	PRO	C-N-CA	-5.42	113.73	120.56
1	C	183	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	B	55	SER	N-CA-C	5.39	119.69	113.38
1	D	206	ALA	N-CA-C	-5.38	104.29	112.04
1	C	51	SER	CA-C-N	-5.38	112.64	122.38
1	C	51	SER	C-N-CA	-5.38	112.64	122.38
1	B	54	GLN	CB-CA-C	-5.37	104.10	111.73
1	C	222	PHE	C-N-CD	5.36	146.99	125.00
1	B	6	ILE	CB-CA-C	-5.36	103.18	110.42
1	B	33	ASP	N-CA-C	5.33	116.14	107.23
1	D	74	GLU	CB-CA-C	-5.32	102.30	110.81
1	B	218	GLN	N-CA-C	-5.31	105.60	111.71
1	C	32	LEU	CA-CB-CG	-5.29	97.78	116.30
1	D	36	GLN	N-CA-C	-5.29	106.86	113.15
1	B	182	ALA	N-CA-C	5.27	117.11	111.36
1	A	161	ASN	N-CA-C	5.27	116.71	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	189	ILE	CB-CA-C	-5.26	104.37	112.05
1	C	195	ILE	CB-CA-C	5.25	119.91	111.29
1	A	93	LEU	N-CA-C	5.25	118.30	109.95
1	B	84	VAL	CB-CA-C	-5.23	105.01	112.22
1	A	1	MET	CA-C-N	5.21	128.95	121.50
1	A	1	MET	C-N-CA	5.21	128.95	121.50
1	D	31	ALA	N-CA-C	5.20	117.21	109.25
1	B	186	ASP	CB-CA-C	-5.20	105.17	111.82
1	B	47	ARG	CA-C-N	5.19	125.17	120.03
1	B	47	ARG	C-N-CA	5.19	125.17	120.03
1	D	185	HIS	N-CA-C	-5.18	106.81	112.72
1	A	47	ARG	CA-C-O	-5.18	114.66	120.25
1	A	59	ILE	CA-C-O	-5.17	115.00	120.48
1	C	60	TYR	N-CA-C	5.17	117.92	109.59
1	D	27	TRP	N-CA-C	5.16	117.20	110.08
1	A	166	ARG	CA-C-N	-5.15	113.62	119.28
1	A	166	ARG	C-N-CA	-5.15	113.62	119.28
1	C	35	VAL	CB-CA-C	-5.13	103.94	112.26
1	C	64	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	C	202	GLU	N-CA-C	5.13	116.68	111.14
1	D	153	LEU	N-CA-C	-5.13	105.60	111.14
1	C	33	ASP	N-CA-C	5.12	115.79	107.23
1	B	216	LEU	CA-C-N	-5.12	113.42	120.28
1	B	216	LEU	C-N-CA	-5.12	113.42	120.28
1	D	154	GLU	N-CA-CB	5.11	117.64	110.12
1	B	167	PRO	N-CA-C	-5.11	106.43	113.53
1	D	11	CYS	CA-C-N	-5.11	114.50	122.37
1	D	11	CYS	C-N-CA	-5.11	114.50	122.37
1	A	71	LEU	CA-C-O	-5.11	114.94	120.81
1	C	140	ALA	N-CA-C	-5.08	105.01	111.11
1	B	10	THR	N-CA-C	5.07	118.57	112.38
1	A	100	ILE	CB-CA-C	-5.06	105.22	111.70
1	D	59	ILE	CA-C-O	-5.06	114.97	120.84
1	C	156	LEU	CA-C-N	-5.05	112.10	120.68
1	C	156	LEU	C-N-CA	-5.05	112.10	120.68
1	B	53	LEU	O-C-N	5.04	129.36	122.46
1	C	216	LEU	CA-CB-CG	-5.04	98.68	116.30
1	B	79	ARG	N-CA-C	5.03	119.61	111.37
1	D	84	VAL	CB-CA-C	-5.02	105.44	112.02
1	A	105	CYS	N-CA-C	-5.01	105.73	111.14
1	C	152	LEU	CA-C-N	-5.01	111.81	121.58
1	C	152	LEU	C-N-CA	-5.01	111.81	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ARG	N-CA-C	5.01	116.02	108.46
1	D	33	ASP	CB-CA-C	-5.01	103.83	110.79

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	181	0
1	B	1815	0	1798	199	1
1	C	1815	0	1797	207	0
1	D	1815	0	1798	202	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	786	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 54.

All (786) 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:HH11	1:B:176:ARG:CB	1.44	1.28
1:B:176:ARG:NH1	1:B:176:ARG:CB	2.07	1.12
1:C:34:ARG:HG2	1:C:34:ARG:HH11	1.15	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ARG:HG3	1:D:149:ARG:HH11	0.99	1.11
1:A:183:ARG:HG3	1:A:183:ARG:HH11	1.11	1.08
1:C:183:ARG:HG3	1:C:183:ARG:HH11	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:B:184:LYS:O	1:B:186:ASP:N	1.88	1.06
1:C:183:ARG:HH11	1:C:183:ARG:CG	1.68	1.06
1:C:151:SER:OG	1:C:154:GLU:HG3	1.53	1.06
1:A:34:ARG:HG2	1:A:34:ARG:HH11	1.17	1.05
1:C:176:ARG:HH11	1:C:176:ARG:CB	1.69	1.05
1:C:183:ARG:HG3	1:C:183:ARG:NH1	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
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:HE21	1:C:224:GLN:N	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:HD12	1:A:187:LEU:H	1.30	0.97
1:A:151:SER:OG	1:A:154:GLU:HG3	1.63	0.96
1:D:224:GLN:N	1:D:224:GLN:HE21	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:N	1:D:209:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:D:34:ARG:HG2	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
1:B:205:GLU:O	1:B:209:ASN:ND2	2.08	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:A:161:ASN:H	1:A:161:ASN:ND2	1.70	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:23:GLN:NE2	1:C:54:GLN:HB3	1.92	0.84
1:C:176:ARG:HB2	1:C:176:ARG:NH1	1.92	0.84
1:C:131:PHE:CD1	1:C:212:LEU:CD1	2.61	0.84
1:A:183:ARG:HG3	1:A:183:ARG:NH1	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:CB	1:C:176:ARG:NH1	2.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ILE:O	1:B:191:GLN:N	2.11	0.82
1:B:25:THR:HG23	1:B:27:TRP:H	1.42	0.81
1:B:224:GLN:HE21	1:B:224:GLN:N	1.77	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:B:223:PRO:C	1:B:224:GLN:HE21	1.87	0.81
1:C:21:ILE:O	1:C:25:THR:HB	1.81	0.81
1:A:176:ARG:NH1	1:A:210:GLU:CD	2.39	0.81
1:B:32:LEU:HD11	1:B:95:LEU:HB3	1.62	0.81
1:B:100:ILE:CD1	1:B:218:GLN:HA	2.10	0.81
1:C:189:ILE:HA	1:C:192:LEU:CD1	2.11	0.81
1:B:209:ASN:HD22	1:B:209:ASN:N	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
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:HG2	1:B:34:ARG:HH11	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:C:75:SER:O	1:C:76:ALA:C	2.26	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:23:GLN:HE22	1:C:54:GLN:HB3	1.48	0.77
1:C:176:ARG:NH1	1:C:210:GLU:OE1	2.17	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:99:SER:O	1:B:103:LEU:HD12	1.84	0.77
1:B:183:ARG:HH11	1:B:183:ARG:HG3	1.50	0.77
1:C:120:VAL:HG21	1:C:225:TRP:CD1	2.20	0.77
1:C:204:ILE:O	1:C:205:GLU:C	2.22	0.77
1:D:145:ILE:O	1:D:146:ARG:HG3	1.85	0.77
1:A:161:ASN:HD22	1:A:161:ASN:N	1.83	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LYS:C	1:B:186:ASP:H	1.94	0.76
1:D:146:ARG:HD3	1:D:149:ARG:CZ	2.16	0.76
1:B:122:ARG:C	1:B:123:LEU:HD23	2.11	0.75
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:B:195:ILE:O	1:B:196:ASP:C	2.28	0.75
1:D:34:ARG:NH1	1:D:71:LEU:O	2.19	0.75
1:B:5:LEU:HD12	1:B:6:ILE:N	2.01	0.74
1:B:7:TYR:CE2	1:B:122:ARG:HD2	2.22	0.74
1:B:223:PRO:C	1:B:224:GLN:NE2	2.45	0.74
1:C:176:ARG:NH1	1:C:210:GLU:CD	2.45	0.74
1:D:5:LEU:HD12	1:D:6:ILE:N	2.02	0.74
1:D:161:ASN:H	1:D:161:ASN:ND2	1.85	0.74
1:A:1:MET:O	1:A:116:PHE:HB3	1.87	0.74
1:B:189:ILE:C	1:B:191:GLN:H	1.95	0.74
1:D:176:ARG:HB3	1:D:176:ARG:HH11	1.52	0.74
1:A:187:LEU:HD12	1:A:187:LEU:N	2.00	0.73
1:C:6:ILE:HD13	1:C:17:MET:HE3	1.70	0.73
1:D:7:TYR:CE2	1:D:122:ARG:HD2	2.23	0.73
1:A:161:ASN:ND2	1:A:161:ASN:N	2.35	0.73
1:B:204:ILE:O	1:B:205:GLU:C	2.27	0.73
1:A:23:GLN:HE22	1:A:54:GLN:HB3	1.53	0.73
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:HA	1:D:219:GLU:OE2	1.87	0.73
1:B:161:ASN:HD22	1:B:161:ASN:H	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:195:ILE:HD12	1:D:195:ILE:C	2.12	0.72
1:D:224:GLN:N	1:D:224:GLN:NE2	2.36	0.72
1:D:224:GLN:H	1:D:224:GLN:NE2	1.87	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD2	1:D:148:ASP:N	2.24	0.70
1:D:184:LYS:HE3	1:D:184:LYS:HA	1.74	0.70
1:B:15:THR:O	1:B:19:ILE:HG13	1.90	0.70
1:B:1:MET:O	1:B:116:PHE:HB3	1.90	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:A:75:SER:O	1:A:76:ALA:C	2.31	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
1:D:199:ARG:O	1:D:200:HIS:C	2.36	0.69
1:A:5:LEU:HD12	1:A:6:ILE:H	1.58	0.69
1:A:32:LEU:HD11	1:A:95:LEU:HB3	1.73	0.69
1:C:122:ARG:C	1:C:123:LEU:HD23	2.17	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:D:122:ARG:C	1:D:123:LEU:HD23	2.16	0.69
1:A:176:ARG:HH11	1:A:210:GLU:CD	2.01	0.68
1:B:192:LEU:N	1:B:193:PRO:HD2	2.07	0.68
1:B:25:THR:CG2	1:B:27:TRP:H	2.07	0.68
1:B:224:GLN:HE21	1:B:224:GLN:CA	2.06	0.68
1:D:179:ILE:O	1:D:182:ALA:N	2.24	0.68
1:A:207:ILE:O	1:A:208:ALA:C	2.36	0.68
1:D:32:LEU:HB2	1:D:97:GLY:HA3	1.73	0.68
1:D:195:ILE:CG2	1:D:200:HIS:HD2	2.06	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:D:145:ILE:C	1:D:146:ARG:HG3	2.19	0.67
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:191:GLN:HA	1:D:191:GLN:NE2	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:49:LEU:CD2	1:A:149:ARG:NH1	2.58	0.67
1:D:179:ILE:O	1:D:180:ARG:C	2.37	0.67
1:D:50:GLU:O	1:D:53:LEU:HB2	1.95	0.66
1:B:123:LEU:HD23	1:B:123:LEU:N	2.08	0.66
1:B:176:ARG:NH1	1:B:176:ARG:HB2	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:OD2	1:A:148:ASP:N	2.26	0.66
1:D:75:SER:O	1:D:76:ALA:C	2.39	0.66
1:A:34:ARG:NH1	1:A:71:LEU:O	2.29	0.66
1:B:176:ARG:HB3	1:B:176:ARG:HH11	0.56	0.66
1:D:34:ARG:HG2	1:D:34:ARG:NH1	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:N	1:C:187:LEU:CD1	2.42	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:D:195:ILE:O	1:D:196:ASP:C	2.40	0.64
1:A:47:ARG:HD2	1:A:60:TYR:CZ	2.32	0.64
1:D:172:ILE:CG2	1:D:175:TYR:HD1	2.11	0.64
1:A:34:ARG:HH11	1:A:34:ARG:CG	1.97	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:5:LEU:HD12	1:C:6:ILE:N	2.13	0.63
1:C:49:LEU:CD2	1:C:149:ARG:CD	2.62	0.63
1:B:34:ARG:HG2	1:B:34:ARG:NH1	2.13	0.63
1:A:15:THR:O	1:A:19:ILE:HG13	1.97	0.63
1:A:100:ILE:HD11	1:A:218:GLN:HA	1.80	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:A:25:THR:HG23	1:A:27:TRP:N	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:106:MET:HB3	1:A:225:TRP:HH2	1.65	0.62
1:A:123:LEU:HD23	1:A:123:LEU:N	2.14	0.62
1:A:145:ILE:O	1:A:146:ARG:HG3	2.00	0.62
1:D:183:ARG:HH11	1:D:183:ARG:CG	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:33:ASP:CG	1:B:36:GLN:HB2	2.26	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:B:145:ILE:C	1:B:146:ARG:HG3	2.26	0.61
1:A:219:GLU:OE2	1:A:219:GLU:HA	1.99	0.61
1:C:210:GLU:O	1:C:213:GLU:HB3	2.01	0.61
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:23:GLN:HE22	1:A:54:GLN:HG3	1.64	0.61
1:A:225:TRP:O	1:A:226:PRO:O	2.19	0.61
1:B:148:ASP:OD2	1:B:148:ASP:N	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:209:ASN:N	1:D:209:ASN:ND2	2.37	0.60
1:A:128:SER:O	1:A:129:ASP:C	2.43	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:A:145:ILE:C	1:A:146:ARG:HG3	2.26	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:A:6:ILE:HD13	1:A:17:MET:HE3	1.84	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:D:6:ILE:HD13	1:D:17:MET:HE3	1.84	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:2:LEU:O	1:D:3:LEU:HD23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:LEU:HD12	1:D:209:ASN:ND2	2.17	0.59
1:A:195:ILE:HG23	1:A:195:ILE:O	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:B:172:ILE:C	1:B:173:ASP:O	2.46	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:A:122:ARG:C	1:A:123:LEU:HD23	2.27	0.58
1:D:220:ARG:HG2	1:D:221:ASP:OD1	2.03	0.58
1:B:169:LEU:C	1:B:171:ASP:H	2.11	0.58
1:A:209:ASN:N	1:A:209:ASN:HD22	2.01	0.58
1:A:87:ARG:HD3	1:A:93:LEU:HD21	1.84	0.58
1:B:189:ILE:C	1:B:191:GLN:N	2.58	0.58
1:C:25:THR:HG23	1:C:27:TRP:CG	2.39	0.58
1:C:189:ILE:C	1:C:192:LEU:HD12	2.28	0.58
1:A:34:ARG:HG2	1:A:71:LEU:O	2.04	0.57
1:B:72:ASP:OD2	1:B:72:ASP:C	2.47	0.57
1:B:179:ILE:O	1:B:179:ILE:HG22	2.03	0.57
1:D:2:LEU:HD12	1:D:3:LEU:H	1.69	0.57
1:D:192:LEU:N	1:D:193:PRO:HD2	2.20	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:D:1:MET:HE3	1:D:116:PHE:HD2	1.69	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:5:LEU:HD12	1:B:6:ILE:H	1.69	0.57
1:B:146:ARG:HD3	1:B:149:ARG:CZ	2.35	0.57
1:B:180:ARG:O	1:B:181:PHE:C	2.48	0.57
1:C:1:MET:O	1:C:116:PHE:HB3	2.05	0.57
1:D:161:ASN:ND2	1:D:161:ASN:N	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:NE2	1:B:224:GLN:CA	2.68	0.56
1:C:87:ARG:HD3	1:C:93:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ASP:HA	1:C:176:ARG:HH12	1.69	0.56
1:C:184:LYS:NZ	1:C:184:LYS:CD	2.65	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:B:209:ASN:ND2	1:B:209:ASN:N	2.42	0.56
1:A:81:ILE:HG22	1:A:82:PHE:N	2.14	0.56
1:A:135:ALA:O	1:A:139:VAL:HG23	2.05	0.56
1:A:1:MET:HE3	1:A:116:PHE:HD2	1.69	0.56
1:B:160:TRP:CE2	1:B:166:ARG:HD3	2.41	0.56
1:D:176:ARG:NH1	1:D:176:ARG:CB	2.69	0.56
1:B:213:GLU:O	1:B:216:LEU:HB2	2.06	0.55
1:C:145:ILE:C	1:C:146:ARG:HG3	2.30	0.55
1:B:75:SER:O	1:B:76:ALA:C	2.50	0.55
1:C:180:ARG:O	1:C:181:PHE:C	2.49	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:B:1:MET:HE3	1:B:116:PHE:CD2	2.42	0.55
1:D:1:MET:HE3	1:D:116:PHE:CD2	2.41	0.55
1:D:169:LEU:C	1:D:171:ASP:H	2.13	0.55
1:D:225:TRP:O	1:D:226:PRO:C	2.50	0.55
1:B:1:MET:HE3	1:B:116:PHE:HD2	1.71	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:42:ALA:HA	1:D:47:ARG:CG	2.37	0.55
1:D:122:ARG:NH2	1:D:219:GLU:OE2	2.40	0.55
1:A:35:VAL:O	1:A:35:VAL:HG12	2.04	0.54
1:B:82:PHE:CD1	1:D:65:PRO:HG3	2.42	0.54
1:B:145:ILE:O	1:B:146:ARG:CG	2.54	0.54
1:D:145:ILE:O	1:D:146:ARG:CG	2.56	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: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:B:6:ILE:HD13	1:B:17:MET:HE3	1.89	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:65:PRO:O	1:B:66:LEU:C	2.48	0.54
1:B:183:ARG:HH11	1:B:183:ARG:HG2	1.73	0.54
1:C:191:GLN:NE2	1:C:191:GLN:HA	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:O	1:C:54:GLN:HB2	2.06	0.54
1:B:50:GLU:O	1:B:53:LEU:HB2	2.07	0.54
1:B:224:GLN:HE21	1:B:224:GLN:HA	1.72	0.54
1:A:204:ILE:O	1:A:205:GLU:C	2.49	0.53
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:D:181:PHE:CZ	1:D:199:ARG:HG2	2.42	0.53
1:D:183:ARG:CG	1:D:183:ARG:NH1	2.71	0.53
1:B:204:ILE:O	1:B:207:ILE:N	2.41	0.53
1:C:224:GLN:HE21	1:C:224:GLN:H	1.48	0.53
1:A:214:HIS:O	1:A:215:ALA:C	2.52	0.53
1:C:128:SER:O	1:C:129:ASP:C	2.50	0.53
1:C:139:VAL:HG21	1:C:207:ILE:HG22	1.91	0.53
1:D:157:ALA:O	1:D:158:GLU:C	2.50	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:A:1:MET:HE3	1:A:116:PHE:CD2	2.44	0.52
1:B:169:LEU:O	1:B:171:ASP:N	2.43	0.52
1:D:2:LEU:HD12	1:D:3:LEU:N	2.23	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:B:169:LEU:C	1:B:171:ASP:N	2.63	0.52
1:C:85:ASP:O	1:C:88:LYS:HG3	2.08	0.52
1:C:32:LEU:HB2	1:C:97:GLY:HA3	1.91	0.52
1:A:183:ARG:CG	1:A:183:ARG:NH1	2.46	0.52
1:D:14:LYS:HZ1	2:D:301:POP:P2	2.31	0.52
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:O	1:B:35:VAL:HG12	2.10	0.52
1:D:33:ASP:OD1	1:D:35:VAL:N	2.43	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:O	1:D:35:VAL:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:VAL:HG22	1:C:70:ILE:HD12	1.92	0.51
1:C:184:LYS:NZ	1:C:184:LYS:CG	2.73	0.51
1:C:132:LEU:CD1	1:C:212:LEU:HD22	2.40	0.51
1:D:181:PHE:CD1	1:D:181:PHE:O	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:C:72:ASP:OD2	1:C:72:ASP:C	2.53	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:D:65:PRO:O	1:D:66:LEU:C	2.53	0.51
1:B:75:SER:C	1:B:77:HIS:N	2.68	0.51
1:D:149:ARG:C	1:D:150:PRO:O	2.45	0.51
1:C:6:ILE:O	1:C:96:GLU:HA	2.11	0.50
1:C:28:PRO:HG2	1:C:93:LEU:HD23	1.91	0.50
1:C:125:LEU:HD22	1:C:215:ALA:HB3	1.94	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:D:176:ARG:NH1	1:D:210:GLU:CD	2.69	0.50
1:D:179:ILE:O	1:D:181:PHE:N	2.44	0.50
1:C:54:GLN:O	1:C:55:SER:HB2	2.11	0.50
1:B:15:THR:HA	1:B:96:GLU:OE1	2.10	0.50
1:B:25:THR:CG2	1:B:27:TRP:CB	2.90	0.50
1:B:32:LEU:CD1	1:B:95:LEU:HB3	2.38	0.50
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:139:VAL:O	1:B:140:ALA:C	2.55	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:D:161:ASN:HD22	1:D:161:ASN:N	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:A:177:CYS:HB2	1:A:210:GLU:CD	2.37	0.50
1:B:205:GLU:O	1:B:206:ALA:C	2.54	0.50
1:C:62:ASP:OD1	1:C:64:ARG:HD2	2.11	0.50
1:D:177:CYS:HB2	1:D:210:GLU:CD	2.35	0.50
1:B:81:ILE:O	1:B:85:ASP:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:O	1:C:56:THR:OG1	2.23	0.50
1:C:127:ASP:O	1:C:128:SER:C	2.54	0.49
1:A:157:ALA:O	1:A:158:GLU:C	2.53	0.49
1:A:224:GLN:H	1:A:224:GLN:HE21	1.58	0.49
1:C:207:ILE:O	1:C:208:ALA:C	2.53	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:38:CYS:O	1:B:41:ILE:HG13	2.12	0.49
1:C:149:ARG:HH11	1:C:149:ARG:CG	2.26	0.49
1:D:169:LEU:C	1:D:171:ASP:N	2.68	0.49
1:D:196:ASP:CG	1:D:196:ASP:O	2.55	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:A:41:ILE:C	1:A:155:GLU:OE2	2.56	0.49
1:C:1:MET:HE3	1:C:116:PHE:CD2	2.48	0.49
1:A:191:GLN:HA	1:A:191:GLN:NE2	2.28	0.48
1:B:33:ASP:OD1	1:B:33:ASP:C	2.54	0.48
1:C:214:HIS:O	1:C:218:GLN:HG3	2.12	0.48
1:A:33:ASP:C	1:A:33:ASP:OD1	2.55	0.48
1:C:1:MET:HE3	1:C:116:PHE:HD2	1.77	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:NE2	1:D:191:GLN:CA	2.72	0.48
1:D:207:ILE:O	1:D:208:ALA:C	2.56	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:35:VAL:C	1:C:37:CYS:H	2.22	0.48
1:C:131:PHE:CE1	1:C:212:LEU:HA	2.49	0.48
1:C:5:LEU:HD12	1:C:6:ILE:H	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:86:TRP:O	1:A:86:TRP:CE3	2.67	0.48
1:A:185:HIS:HB2	1:A:187:LEU:HD11	1.96	0.48
1:B:2:LEU:HD12	1:B:3:LEU:H	1.79	0.48
1:B:176:ARG:NH1	1:B:210:GLU:OE1	2.46	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:35:VAL:HA	1:C:70:ILE:CD1	2.43	0.48
1:C:199:ARG:HA	1:C:202:GLU:HG3	1.96	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:127:ASP:O	1:B:128:SER:C	2.57	0.47
1:D:14:LYS:O	1:D:15:THR:C	2.57	0.47
1:C:214:HIS:C	1:C:216:LEU:N	2.68	0.47
1:B:32:LEU:HA	1:B:32:LEU:HD23	1.38	0.47
1:C:184:LYS:HE3	1:C:184:LYS:HB2	1.81	0.47
1:A:176:ARG:HH12	1:A:210:GLU:CD	2.19	0.47
1:B:225:TRP:HA	1:B:226:PRO:HD2	1.50	0.47
1:D:47:ARG:HB3	1:D:60:TYR:OH	2.14	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:B:32:LEU:HB2	1:B:97:GLY:CA	2.43	0.47
1:B:50:GLU:OE1	1:D:57:ARG:NE	2.48	0.47
1:D:48:PRO:HB2	1:D:52:GLU:HG3	1.96	0.47
1:D:209:ASN:O	1:D:212:LEU:HB3	2.14	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:166:ARG:O	1:C:167:PRO:C	2.53	0.46
1:D:23:GLN:HE22	1:D:54:GLN:CB	2.28	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
1:D:49:LEU:H	1:D:52:GLU:CG	2.28	0.46
1:A:192:LEU:HD23	1:A:192:LEU:HA	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:O	1:A:196:ASP:C	2.59	0.46
1:B:9:PRO:HB3	1:B:215:ALA:HB1	1.98	0.46
1:B:85:ASP:O	1:B:88:LYS:HG3	2.15	0.46
1:B:124:ARG:CG	1:B:124:ARG:HH11	2.28	0.46
1:C:177:CYS:SG	1:C:207:ILE:HG13	2.55	0.46
1:C:191:GLN:C	1:C:193:PRO:HD2	2.41	0.46
1:A:34:ARG:O	1:A:37:CYS:HB2	2.16	0.46
1:A:156:LEU:HD13	1:A:175:TYR:CD2	2.41	0.46
1:D:128:SER:O	1:D:129:ASP:C	2.57	0.46
1:A:217:SER:O	1:A:218:GLN:C	2.57	0.45
1:B:34:ARG:NH1	1:B:34:ARG:CG	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: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:B:65:PRO:HB2	1:B:68:GLU:HG2	1.98	0.45
1:A:17:MET:O	1:A:20:GLN:HB2	2.16	0.45
1:A:147:GLU:H	1:A:147:GLU:HG3	1.60	0.45
1:B:204:ILE:HG22	1:B:205:GLU:N	2.31	0.45
1:A:14:LYS:O	1:A:15:THR:C	2.59	0.45
1:B:22:ALA:HA	1:B:25:THR:HG22	1.98	0.45
1:C:33:ASP:CG	1:C:36:GLN:HB2	2.42	0.45
1:A:4:HIS:CE1	1:A:21:ILE:HD13	2.51	0.45
1:B:6:ILE:O	1:B:96:GLU:HA	2.16	0.45
1:B:161:ASN:ND2	1:B:161:ASN:N	2.63	0.45
1:D:34:ARG:HH12	1:D:72:ASP:HA	1.82	0.45
1:D:109:SER:HA	1:D:110:PRO:HD3	1.72	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
1:C:182:ALA:C	1:C:184:LYS:H	2.24	0.45
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:B:169:LEU:O	1:B:170:GLU:C	2.60	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:61:LEU:O	1:A:62:ASP:CB	2.65	0.44
1:A:212:LEU:HA	1:A:212:LEU:HD12	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:146:ARG:HD3	1:B:149:ARG:NE	2.32	0.44
1:B:184:LYS:O	1:B:185:HIS:C	2.52	0.44
1:B:184:LYS:C	1:B:186:ASP:N	2.52	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:225:TRP:HA	1:D:226:PRO:HD2	1.76	0.44
1:A:66:LEU:HD22	1:A:66:LEU:HA	1.78	0.44
1:A:173:ASP:HA	1:A:176:ARG:HH22	1.83	0.44
1:B:74:GLU:OE1	1:B:74:GLU:HA	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:HD23	1:C:153:LEU:HA	1.72	0.44
1:B:157:ALA:O	1:B:158:GLU:C	2.61	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:34:ARG:NH1	1:B:72:ASP:C	2.76	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:66:LEU:HD13	1:A:66:LEU:C	2.43	0.44
1:A:131:PHE:HD1	1:A:212:LEU:HD13	1.76	0.44
1:B:3:LEU:HD23	1:B:3:LEU:HA	1.71	0.44
1:C:96:GLU:OE2	1:C:97:GLY:HA2	2.17	0.44
1:C:131:PHE:HA	1:C:134:ARG:NH1	2.33	0.44
1:D:29:VAL:HA	1:D:94:ILE:HB	2.00	0.44
1:A:5:LEU:HD12	1:A:95:LEU:O	2.18	0.44
1:A:131:PHE:HA	1:A:134:ARG:NH1	2.32	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: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:A:138:ARG:HG3	1:A:142:MET:HE3	2.00	0.43
1:B:62:ASP:HB2	1:B:79:ARG:NH1	2.33	0.43
1:C:139:VAL:O	1:C:140:ALA:C	2.60	0.43
1:C:225:TRP:HA	1:C:226:PRO:HD2	1.60	0.43
1:D:191:GLN:CA	1:D:191:GLN:HE21	2.31	0.43
1:A:32:LEU:HA	1:A:32:LEU:HD23	1.17	0.43
1:A:172:ILE:HG22	1:A:173:ASP:O	2.18	0.43
1:C:38:CYS:O	1:C:41:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE21	1:D:40:GLN:HB3	1.56	0.43
1:B:14:LYS:O	1:B:15:THR:C	2.60	0.43
1:B:27:TRP:CD1	1:B:27:TRP:N	2.85	0.43
1:D:212:LEU:C	1:D:212:LEU:HD12	2.44	0.43
1:B:131:PHE:CE1	1:B:212:LEU:HA	2.54	0.43
1:B:137:GLN:NE2	1:B:141:GLU:OE1	2.35	0.43
1:D:35:VAL:C	1:D:37:CYS:H	2.27	0.43
1:B:36:GLN:HG3	1:B:45:SER:O	2.19	0.43
1:B:131:PHE:O	1:B:132:LEU:C	2.61	0.43
1:D:43:THR:OG1	1:D:149:ARG:HD3	2.17	0.43
1:A:124:ARG:HH11	1:A:124:ARG:CG	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:C:43:THR:HB	1:C:155:GLU:CD	2.44	0.43
1:D:220:ARG:C	1:D:221:ASP:OD1	2.62	0.43
1:A:35:VAL:HG22	1:A:70:ILE:HD12	2.01	0.43
1:A:181:PHE:CD1	1:A:181:PHE:C	2.97	0.43
1:B:53:LEU:O	1:B:54:GLN:HB2	2.18	0.43
1:B:176:ARG:CB	1:B:176:ARG:CZ	2.80	0.43
1:C:145:ILE:CG2	1:C:146:ARG:N	2.82	0.43
1:C:34:ARG:HH12	1:C:72:ASP:HA	1.84	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:B:200:HIS:O	1:B:203:LEU:HB3	2.19	0.43
1:D:80:LEU:HD12	1:D:80:LEU:HA	1.61	0.43
1:B:34:ARG:O	1:B:37:CYS:HB2	2.19	0.43
1:C:61:LEU:HA	1:C:61:LEU:HD23	1.76	0.43
1:C:153:LEU:O	1:C:156:LEU:HB3	2.19	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:HA	1:C:32:LEU:HD23	1.33	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLY:HA3	1:B:175:TYR:CZ	2.52	0.42
1:B:109:SER:HA	1:B:110:PRO:HD3	1.66	0.42
1:B:191:GLN:C	1:B:193:PRO:HD2	2.43	0.42
1:C:14:LYS:NZ	2:C:301:POP:O	2.42	0.42
1:B:84:VAL:O	1:B:85:ASP:C	2.58	0.42
1:D:6:ILE:O	1:D:96:GLU:HA	2.19	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:A:153:LEU:HD22	1:A:192:LEU:HB3	2.01	0.42
1:B:191:GLN:HA	1:B:191:GLN:NE2	2.34	0.42
1:C:80:LEU:HD12	1:C:80:LEU:HA	1.78	0.42
1:C:125:LEU:HD22	1:C:215:ALA:CB	2.49	0.42
1:C:212:LEU:HA	1:C:212:LEU:HD12	1.67	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:CB	1:D:176:ARG:CZ	2.97	0.42
1:A:48:PRO:HB2	1:A:52:GLU:HG3	2.02	0.42
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.78	0.42
1:C:170:GLU:O	1:C:176:ARG:HG3	2.19	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:A:139:VAL:O	1:A:140:ALA:C	2.63	0.42
1:B:23:GLN:HE22	1:B:54:GLN:HG3	1.85	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:C:61:LEU:O	1:C:62:ASP:CB	2.64	0.42
1:D:72:ASP:C	1:D:72:ASP:OD2	2.63	0.42
1:A:204:ILE:O	1:A:206:ALA:N	2.53	0.42
1:C:224:GLN:N	1:C:224:GLN:NE2	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:204:ILE:C	1:A:206:ALA:N	2.78	0.41
1:A:212:LEU:O	1:A:212:LEU:HD12	2.20	0.41
1:D:35:VAL:O	1:D:35:VAL:CG1	2.64	0.41
1:D:66:LEU:C	1:D:66:LEU:HD13	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:LYS:HD2	1:D:123:LEU:CD2	2.50	0.41
1:C:17:MET:O	1:C:20:GLN:HB2	2.21	0.41
1:C:149:ARG:HA	1:C:150:PRO:HD2	1.85	0.41
1:D:50:GLU:HA	1:D:53:LEU:HD12	2.02	0.41
1:D:220:ARG:CG	1:D:221:ASP:OD1	2.67	0.41
1:A:20:GLN:O	1:A:21:ILE:C	2.60	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:C:165:ALA:O	1:C:169:LEU:HG	2.21	0.41
1:C:209:ASN:ND2	1:C:209:ASN:H	2.17	0.41
1:D:70:ILE:O	1:D:71:LEU:C	2.61	0.41
1:B:14:LYS:N	2:B:301:POP:O5	2.46	0.41
1:B:35:VAL:C	1:B:37:CYS:H	2.28	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:28:PRO:HG2	1:A:93:LEU:HD22	2.01	0.41
1:A:162:TYR:CD2	1:A:162:TYR:N	2.89	0.41
1:A:172:ILE:O	1:A:173:ASP:O	2.37	0.41
1:C:14:LYS:O	1:C:15:THR:C	2.63	0.41
1:C:62:ASP:HB2	1:C:79:ARG:NH1	2.35	0.41
1:C:109:SER:HA	1:C:110:PRO:HD3	1.64	0.41
1:D:75:SER:C	1:D:77:HIS:N	2.79	0.41
1:D:165:ALA:O	1:D:166:ARG:C	2.62	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:B:110:PRO:O	1:B:111:PHE:C	2.63	0.41
1:C:176:ARG:O	1:C:177:CYS:C	2.63	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:64:ARG:HA	1:A:65:PRO:HD3	1.89	0.41
1:A:179:ILE:O	1:A:182:ALA:N	2.54	0.41
1:A:191:GLN:O	1:A:192:LEU:C	2.64	0.41
1:B:14:LYS:HZ1	2:B:301:POP:P2	2.43	0.41
1:B:34:ARG:NH1	1:B:73:ALA:N	2.69	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:210:GLU:O	1:B:210:GLU:HG3	2.21	0.41
1:C:5:LEU:HD12	1:C:95:LEU:O	2.21	0.41
1:C:40:GLN:HE21	1:C:40:GLN:HB3	1.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:GLN:O	1:C:141:GLU:HG3	2.21	0.41
1:C:165:ALA:O	1:C:169:LEU:N	2.34	0.41
1:D:3:LEU:HD23	1:D:3:LEU:HA	1.74	0.41
1:D:43:THR:OG1	1:D:149:ARG:CD	2.68	0.41
1:B:196:ASP:N	1:B:196:ASP:OD2	2.54	0.41
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.66	0.41
1:C:138:ARG:HG3	1:C:142:MET:HE3	2.03	0.41
1:C:212:LEU:HB3	1:C:213:GLU:H	1.70	0.41
1:D:35:VAL:HG12	1:D:45:SER:HB2	2.02	0.41
1:D:156:LEU:CD2	1:D:189:ILE:CG2	2.99	0.41
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:120:VAL:HG21	1:A:225:TRP:HD1	1.86	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:5:LEU:HD12	1:B:5:LEU:C	2.43	0.40
1:B:20:GLN:HE21	1:B:20:GLN:HB3	1.79	0.40
1:B:199:ARG:HA	1:B:202:GLU:OE2	2.22	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:C:214:HIS:O	1:C:215:ALA:C	2.62	0.40
1:D:124:ARG:HD2	1:D:219:GLU:OE1	2.21	0.40
1:D:195:ILE:CG2	1:D:200:HIS:CD2	2.97	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:169:LEU:C	1:C:171:ASP:N	2.76	0.40
1:C:195:ILE:O	1:C:196:ASP:C	2.65	0.40
1:D:25:THR:CG2	1:D:27:TRP:CG	3.02	0.40
1:D:41:ILE:O	1:D:42:ALA:C	2.65	0.40
1:D:144:ALA:HB3	1:D:149:ARG:NH2	2.37	0.40
1:D:218:GLN:O	1:D:219:GLU:C	2.63	0.40
1:A:3:LEU:HD23	1:A:3:LEU:HA	1.55	0.40
1:A:94:ILE:H	1:A:94:ILE:HG13	1.66	0.40
1:A:149:ARG:C	1:A:150:PRO:O	2.64	0.40
1:A:192:LEU:N	1:A:193:PRO:HD2	2.37	0.40
1:C:75:SER:C	1:C:77:HIS:N	2.76	0.40
1:A:34:ARG:HH12	1:A:72:ASP:HA	1.87	0.40
1:A:64:ARG:HH11	1:A:64:ARG:HD2	1.53	0.40
1:A:176:ARG:NH1	1:A:210:GLU:OE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ILE:HG12	1:C:111:PHE:CD2	2.57	0.40
1:D:185:HIS:O	1:D:186:ASP:C	2.64	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 [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	224/253 (88%)	185 (83%)	31 (14%)	8 (4%)	2	10
1	B	224/253 (88%)	180 (80%)	30 (13%)	14 (6%)	1	3
1	C	224/253 (88%)	183 (82%)	32 (14%)	9 (4%)	2	8
1	D	224/253 (88%)	191 (85%)	21 (9%)	12 (5%)	1	4
All	All	896/1012 (88%)	739 (82%)	114 (13%)	43 (5%)	2	6

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

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Mol	Chain	Res	Type
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
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%)	145 (76%)	47 (24%)	1	2
1	B	192/215 (89%)	142 (74%)	50 (26%)	0	2
1	C	192/215 (89%)	144 (75%)	48 (25%)	0	2
1	D	192/215 (89%)	144 (75%)	48 (25%)	0	2
All	All	768/860 (89%)	575 (75%)	193 (25%)	0	2

All (193) 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	41	ILE
1	A	47	ARG
1	A	62	ASP
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	123	LEU
1	A	124	ARG
1	A	132	LEU
1	A	148	ASP
1	A	159	LEU

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Mol	Chain	Res	Type
1	A	161	ASN
1	A	168	ILE
1	A	171	ASP
1	A	181	PHE
1	A	183	ARG
1	A	187	LEU
1	A	189	ILE
1	A	190	SER
1	A	191	GLN
1	A	194	ASN
1	A	195	ILE
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	37	CYS
1	B	40	GLN
1	B	41	ILE
1	B	47	ARG
1	B	52	GLU
1	B	59	ILE
1	B	62	ASP
1	B	65	PRO
1	B	66	LEU
1	B	68	GLU
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

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Mol	Chain	Res	Type
1	B	123	LEU
1	B	124	ARG
1	B	132	LEU
1	B	148	ASP
1	B	151	SER
1	B	159	LEU
1	B	161	ASN
1	B	169	LEU
1	B	171	ASP
1	B	172	ILE
1	B	176	ARG
1	B	180	ARG
1	B	183	ARG
1	B	192	LEU
1	B	194	ASN
1	B	195	ILE
1	B	200	HIS
1	B	201	VAL
1	B	207	ILE
1	B	209	ASN
1	B	210	GLU
1	B	218	GLN
1	B	220	ARG
1	B	224	GLN
1	C	2	LEU
1	C	12	SER
1	C	19	ILE
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	68	GLU
1	C	70	ILE
1	C	74	GLU
1	C	75	SER

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Mol	Chain	Res	Type
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	123	LEU
1	C	124	ARG
1	C	132	LEU
1	C	148	ASP
1	C	149	ARG
1	C	156	LEU
1	C	168	ILE
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	207	ILE
1	C	216	LEU
1	C	224	GLN
1	D	2	LEU
1	D	12	SER
1	D	19	ILE
1	D	20	GLN
1	D	23	GLN
1	D	25	THR
1	D	34	ARG
1	D	40	GLN
1	D	41	ILE
1	D	47	ARG
1	D	62	ASP
1	D	65	PRO

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Mol	Chain	Res	Type
1	D	66	LEU
1	D	68	GLU
1	D	70	ILE
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	116	PHE
1	D	117	GLN
1	D	119	HIS
1	D	123	LEU
1	D	124	ARG
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	187	LEU
1	D	191	GLN
1	D	195	ILE
1	D	200	HIS
1	D	202	GLU
1	D	209	ASN
1	D	213	GLU
1	D	216	LEU
1	D	220	ARG
1	D	224	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	20	GLN

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Mol	Chain	Res	Type
1	A	23	GLN
1	A	40	GLN
1	A	161	ASN
1	A	194	ASN
1	A	200	HIS
1	A	209	ASN
1	A	224	GLN
1	B	4	HIS
1	B	23	GLN
1	B	40	GLN
1	B	161	ASN
1	B	191	GLN
1	B	200	HIS
1	B	209	ASN
1	B	224	GLN
1	C	4	HIS
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	161	ASN
1	D	191	GLN
1	D	200	HIS
1	D	209	ASN
1	D	224	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	POP	C	301	-	6,8,8	1.67	2 (33%)	12,13,13	2.28	4 (33%)
2	POP	B	301	-	6,8,8	1.65	1 (16%)	12,13,13	1.47	2 (16%)
2	POP	D	301	-	6,8,8	1.59	1 (16%)	12,13,13	2.15	5 (41%)
2	POP	A	301	-	6,8,8	1.14	0	12,13,13	1.54	2 (16%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	POP	P1-O1	3.23	1.60	1.50
2	D	301	POP	P1-O1	3.08	1.60	1.50
2	C	301	POP	P1-O1	2.37	1.57	1.50
2	C	301	POP	P2-O6	-2.10	1.47	1.54

All (13) 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	4.18	123.49	107.80
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	2.68	117.84	107.80
2	D	301	POP	O6-P2-O5	2.64	117.70	107.80
2	B	301	POP	O3-P1-O2	2.44	116.95	107.80
2	D	301	POP	O5-P2-O	-2.34	96.78	104.64
2	C	301	POP	O2-P1-O1	-2.30	101.87	110.83
2	C	301	POP	O-P1-O1	-2.13	99.81	111.04
2	D	301	POP	O2-P1-O	-2.07	97.68	104.64
2	A	301	POP	O6-P2-O5	2.04	115.46	107.80

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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	226/253 (89%)	-0.64	0 100 100	65, 85, 105, 112	0
1	B	226/253 (89%)	-0.63	0 100 100	65, 85, 104, 111	0
1	C	226/253 (89%)	-0.69	0 100 100	65, 85, 105, 111	0
1	D	226/253 (89%)	-0.56	1 (0%) 88 84	65, 85, 104, 112	0
All	All	904/1012 (89%)	-0.63	1 (0%) 92 90	65, 85, 105, 112	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	12	SER	2.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	POP	D	301	9/9	0.93	0.09	83,86,87,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	POP	C	301	9/9	0.94	0.09	92,94,98,99	0
2	POP	B	301	9/9	0.96	0.06	89,89,92,92	0
2	POP	A	301	9/9	0.97	0.06	89,90,91,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.