



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:16 AM UTC

PDB ID : 2NVU / pdb_00002nvu
Title : Structure of APPBP1-UBA3 NEDD8-NEDD8-MgATP-Ubc12(C111A), a trapped ubiquitin-like protein activation complex
Authors : Huang, D.T.; Hunt, H.W.; Zhuang, M.; Ohi, M.D.; Holton, J.M.; Schulman, B.A.
Deposited on : 2006-11-13
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

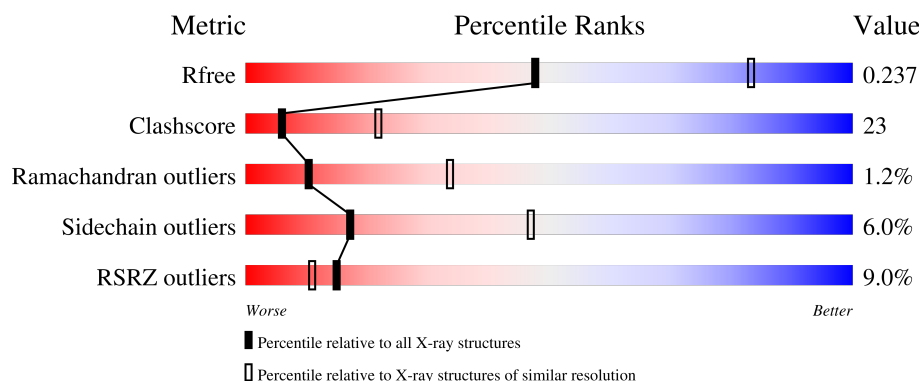
1 Overall quality at a glance

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	536	 2% 60% 35% . .
2	B	805	 11% 54% 38% 6% .
3	C	180	 66% 28% . .
4	I	81	 60% 28% 5% 6%

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Mol	Chain	Length	Quality of chain
4	J	81	60% 27% 51% 15% • 6%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13090 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 NEDD8-activating enzyme E1 regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4212	2664	719	813	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP Q13564
A	0	SER	-	cloning artifact	UNP Q13564

- Molecule 2 is a protein called Maltose binding protein/NEDD8-activating enzyme E1 catalytic subunit chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	789	Total	C	N	O	S	0	0	0
			6174	3957	1026	1167	24			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	998	MET	-	SEE REMARK 999	UNP Q8TBC4
B	999	LYS	-	SEE REMARK 999	UNP Q8TBC4
B	1000	LEU	-	SEE REMARK 999	UNP Q8TBC4
B	1001	MET	-	SEE REMARK 999	UNP Q8TBC4
B	1371	ALA	-	SEE REMARK 999	UNP Q8TBC4

- Molecule 3 is a protein called NEDD8-conjugating enzyme Ubc12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	176	Total	C	N	O	S	4	0	0
			1427	912	241	268	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	cloning artifact	UNP P61081
C	0	SER	-	cloning artifact	UNP P61081
C	?	-	SER	deletion	UNP P61081
C	?	-	ALA	deletion	UNP P61081
C	?	-	GLY	deletion	UNP P61081
C	?	-	GLY	deletion	UNP P61081
C	?	-	THR	deletion	UNP P61081
C	111	ALA	CYS	engineered mutation	UNP P61081

- Molecule 4 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	76	Total	C	N	O	S	0	0	0
			600	378	104	116	2			
4	J	76	Total	C	N	O	S	0	0	0
			599	378	104	115	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	GLY	-	cloning artifact	UNP Q15843
I	-3	SER	-	cloning artifact	UNP Q15843
I	-2	GLY	-	cloning artifact	UNP Q15843
I	-1	GLY	-	cloning artifact	UNP Q15843
I	0	SER	-	cloning artifact	UNP Q15843
J	-4	GLY	-	cloning artifact	UNP Q15843
J	-3	SER	-	cloning artifact	UNP Q15843
J	-2	GLY	-	cloning artifact	UNP Q15843
J	-1	GLY	-	cloning artifact	UNP Q15843
J	0	SER	-	cloning artifact	UNP Q15843

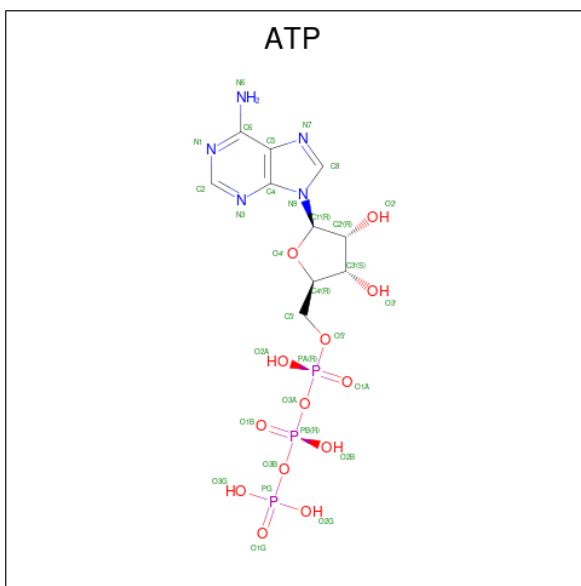
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

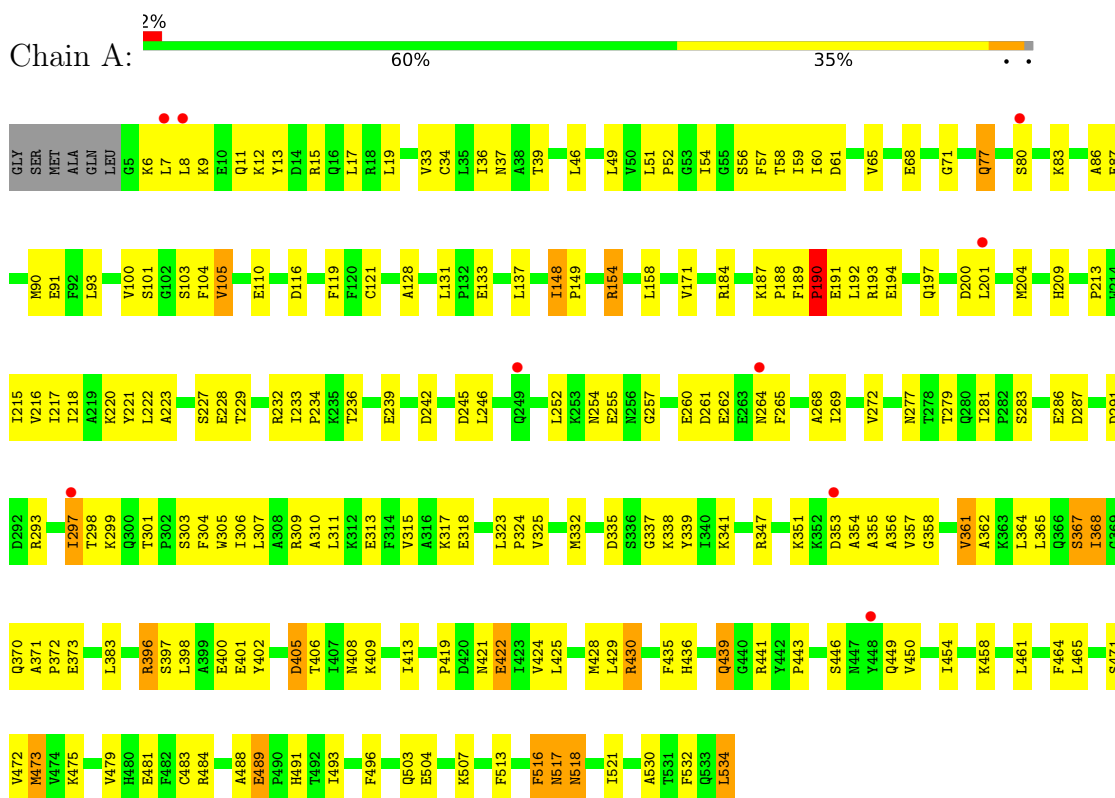
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	11	Total O 11 11	0	0
8	B	27	Total O 27 27	0	0
8	C	4	Total O 4 4	0	0
8	I	3	Total O 3 3	0	0

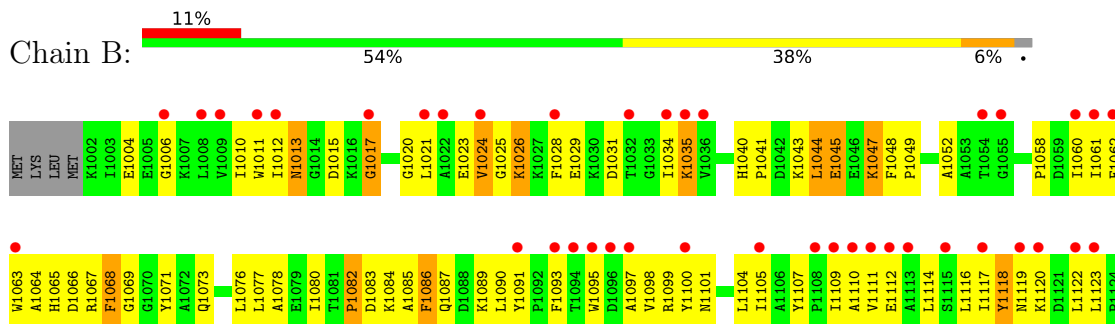
3 Residue-property plots

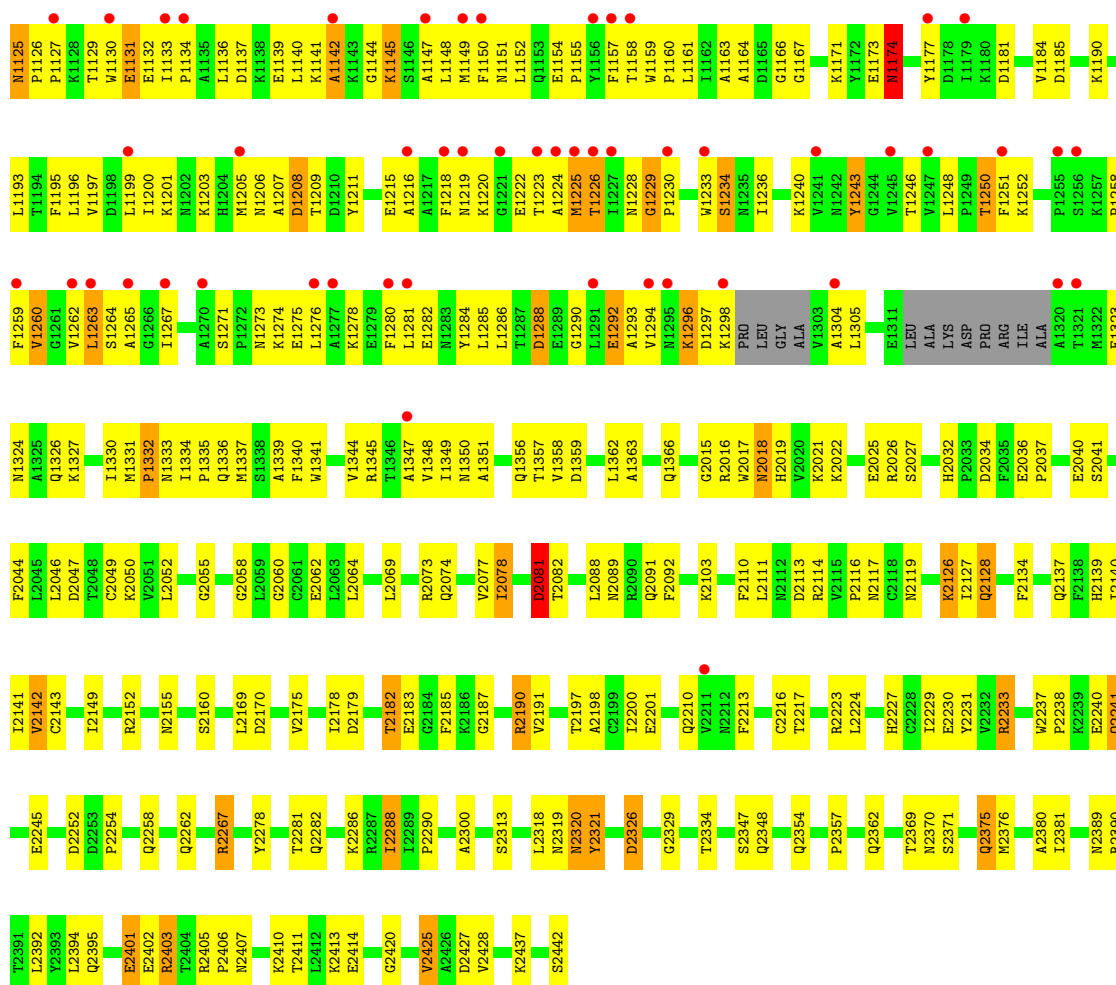
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit



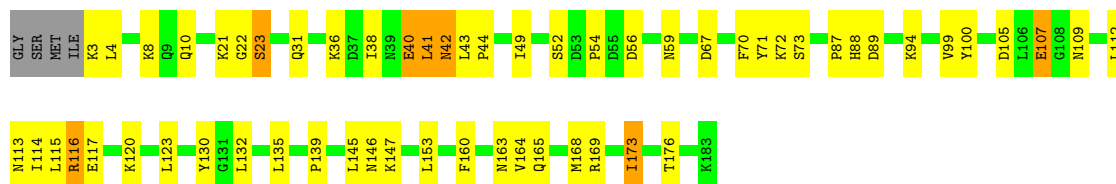
• Molecule 2: Maltose binding protein/NEDD8-activating enzyme E1 catalytic subunit chimera





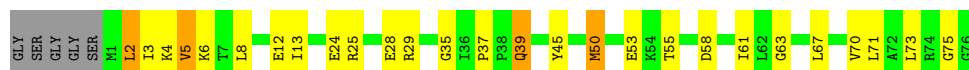
• Molecule 3: NEDD8-conjugating enzyme Ubc12

Chain C: 66% 28%



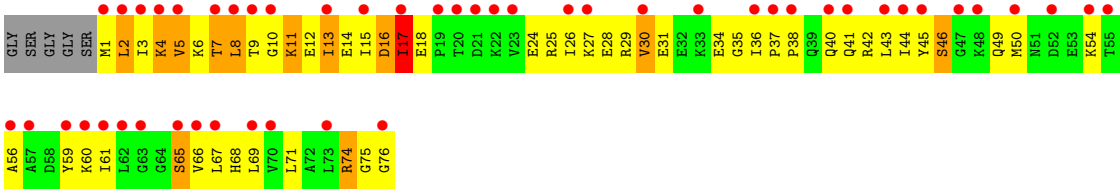
• Molecule 4: NEDD8

Chain I: 60% 28% 5% 6%



• Molecule 4: NEDD8

Chain J: 27% 51% 15% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.49Å 156.49Å 190.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.80) 98.6 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.274 0.241 , 0.237	Depositor DCC
R_{free} test set	3561 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13090	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/4294	1.01	21/5807 (0.4%)
2	B	0.53	0/6318	1.06	39/8586 (0.5%)
3	C	0.49	0/1458	0.97	5/1963 (0.3%)
4	I	0.55	0/605	1.02	1/808 (0.1%)
4	J	0.56	0/604	1.27	8/808 (1.0%)
All	All	0.52	0/13279	1.04	74/17972 (0.4%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	30	VAL	N-CA-C	-11.79	96.31	111.05
4	J	8	LEU	N-CA-C	9.72	122.89	111.02
2	B	1234	SER	N-CA-C	8.92	120.77	111.14
2	B	1260	VAL	N-CA-C	8.07	119.51	107.80
1	A	517	ASN	N-CA-C	7.82	122.41	113.02
3	C	173	ILE	N-CA-C	-7.61	96.51	107.77
2	B	2288	ILE	N-CA-C	7.50	119.26	109.58
2	B	2320	ASN	N-CA-C	7.47	126.72	110.80
4	J	13	ILE	N-CA-C	7.08	118.67	107.98
2	B	1125	ASN	CA-C-N	-7.02	113.15	120.38
2	B	1125	ASN	C-N-CA	-7.02	113.15	120.38
2	B	1288	ASP	N-CA-C	-6.97	104.91	113.41
1	A	472	VAL	N-CA-C	6.91	119.59	109.63
1	A	257	GLY	N-CA-C	-6.78	105.39	114.95
2	B	1348	VAL	N-CA-C	-6.74	105.77	111.56
2	B	2081	ASP	N-CA-C	6.74	120.36	110.59
1	A	148	ILE	N-CA-C	6.68	115.17	107.89
2	B	2047	ASP	N-CA-C	6.66	122.07	113.88
4	J	7	THR	N-CA-C	-6.58	99.80	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2321	TYR	N-CA-C	6.56	120.22	109.06
1	A	148	ILE	CA-C-N	6.42	127.87	119.84
1	A	148	ILE	C-N-CA	6.42	127.87	119.84
2	B	2403	ARG	N-CA-C	6.40	120.69	113.01
2	B	1024	VAL	N-CA-C	-6.39	105.46	112.80
2	B	1225	MET	N-CA-C	6.37	118.75	109.07
2	B	1229	GLY	CA-C-N	6.29	125.98	119.82
2	B	1229	GLY	C-N-CA	6.29	125.98	119.82
1	A	306	ILE	N-CA-C	-6.16	104.74	110.53
4	I	50	MET	N-CA-C	6.10	119.05	109.96
2	B	2326	ASP	N-CA-C	6.09	118.22	110.61
3	C	107	GLU	N-CA-C	-6.08	105.90	113.38
1	A	39	THR	N-CA-C	-6.06	101.22	109.95
3	C	145	LEU	N-CA-C	-6.06	105.93	113.38
2	B	2088	LEU	N-CA-C	6.00	120.33	113.19
1	A	17	LEU	N-CA-C	-5.99	104.87	111.82
4	J	17	ILE	N-CA-C	5.88	118.65	108.95
2	B	1334	ILE	CA-C-N	5.79	125.16	118.85
2	B	1334	ILE	C-N-CA	5.79	125.16	118.85
1	A	489	GLU	CA-C-N	5.78	126.08	119.83
1	A	489	GLU	C-N-CA	5.78	126.08	119.83
3	C	89	ASP	N-CA-C	-5.75	102.92	110.39
2	B	1035	LYS	N-CA-C	5.72	118.95	110.48
1	A	534	LEU	N-CA-C	5.72	127.01	111.00
1	A	362	ALA	N-CA-C	-5.70	105.15	111.71
2	B	1142	ALA	N-CA-C	-5.68	106.20	113.01
2	B	2143	CYS	N-CA-C	5.66	118.63	109.40
2	B	1120	LYS	N-CA-C	5.63	117.86	111.11
2	B	1069	GLY	N-CA-C	-5.57	105.64	112.77
2	B	2267	ARG	N-CA-C	-5.56	105.22	111.28
4	J	11	LYS	N-CA-C	5.56	117.58	108.52
2	B	2413	LYS	N-CA-C	-5.53	105.27	112.23
2	B	2319	ASN	CA-C-N	5.51	132.07	121.54
2	B	2319	ASN	C-N-CA	5.51	132.07	121.54
2	B	1013	ASN	N-CA-C	5.51	117.98	110.55
1	A	7	LEU	N-CA-C	-5.49	106.66	113.19
4	J	65	SER	N-CA-C	5.49	117.67	108.73
2	B	1091	TYR	CA-C-N	5.43	125.10	119.56
2	B	1091	TYR	C-N-CA	5.43	125.10	119.56
3	C	40	GLU	N-CA-C	-5.43	105.97	112.59
1	A	242	ASP	N-CA-C	-5.42	105.07	110.97
2	B	2329	GLY	N-CA-C	-5.30	100.71	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	CYS	N-CA-C	-5.27	105.62	111.36
1	A	367	SER	N-CA-C	-5.26	106.80	114.12
1	A	368	ILE	N-CA-C	-5.21	108.43	113.53
4	J	30	VAL	CB-CA-C	-5.20	104.11	112.16
1	A	491	HIS	N-CA-C	5.18	117.60	111.33
2	B	2036	GLU	CA-C-N	5.16	125.16	119.90
2	B	2036	GLU	C-N-CA	5.16	125.16	119.90
2	B	2175	VAL	N-CA-C	-5.14	103.06	108.15
2	B	2126	LYS	N-CA-C	-5.13	101.35	109.76
1	A	396	ARG	N-CA-C	-5.11	103.79	110.53
2	B	1184	VAL	N-CA-C	-5.11	108.30	113.20
2	B	1363	ALA	N-CA-C	-5.05	105.67	111.07
1	A	361	VAL	N-CA-C	-5.03	106.25	111.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4212	0	4160	169	0
2	B	6174	0	6117	303	0
3	C	1427	0	1427	39	0
4	I	600	0	638	29	0
4	J	599	0	638	79	0
5	B	1	0	0	0	0
6	B	1	0	0	0	0
7	B	31	0	12	5	0
8	A	11	0	0	0	0
8	B	27	0	0	0	0
8	C	4	0	0	0	0
8	I	3	0	0	0	0
All	All	13090	0	12992	594	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (594) 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)
4:J:15:ILE:HG23	4:J:29:ARG:HD2	1.24	1.10
1:A:46:LEU:HD23	1:A:93:LEU:HD13	1.27	1.09
4:J:5:VAL:HG22	4:J:13:ILE:HG22	1.42	1.01
4:J:31:GLU:HB2	4:J:36:ILE:O	1.66	0.95
1:A:297:ILE:HD13	1:A:297:ILE:H	1.28	0.95
2:B:1215:GLU:HG2	2:B:1219:ASN:HD21	1.33	0.94
2:B:2064:LEU:HB3	2:B:2111:LEU:HD22	1.48	0.94
4:J:15:ILE:CG2	4:J:29:ARG:HD2	1.97	0.93
1:A:46:LEU:HD23	1:A:93:LEU:CD1	2.01	0.91
2:B:1045:GLU:HG2	2:B:1063:TRP:CH2	2.07	0.89
2:B:1045:GLU:HG2	2:B:1063:TRP:CZ2	2.08	0.89
4:J:31:GLU:O	4:J:35:GLY:HA2	1.73	0.88
2:B:1193:LEU:HD23	2:B:1358:VAL:HG13	1.54	0.87
2:B:1041:PRO:HG2	2:B:1044:LEU:HB3	1.57	0.86
1:A:365:LEU:HD12	1:A:372:PRO:HA	1.56	0.84
1:A:311:LEU:HD11	1:A:383:LEU:HD11	1.57	0.84
2:B:1049:PRO:HG3	2:B:1071:TYR:HE1	1.43	0.83
2:B:1006:GLY:O	2:B:1034:ILE:HG23	1.78	0.83
1:A:396:ARG:HH12	1:A:408:ASN:HB2	1.44	0.82
2:B:1282:GLU:HA	2:B:1286:LEU:HD12	1.62	0.82
1:A:8:LEU:HA	1:A:11:GLN:HE21	1.44	0.81
4:I:55:THR:HG22	4:I:58:ASP:OD2	1.81	0.81
1:A:261:ASP:HB3	4:J:74:ARG:NH2	1.96	0.81
2:B:1012:ILE:HG13	2:B:1062:PHE:HB2	1.63	0.80
2:B:1109:ILE:HB	2:B:1263:LEU:HG	1.62	0.80
1:A:518:ASN:HB3	1:A:532:PHE:O	1.82	0.80
2:B:1260:VAL:HB	2:B:1330:ILE:HA	1.64	0.79
2:B:1110:ALA:HB3	2:B:1263:LEU:HD23	1.65	0.79
4:I:2:LEU:HD12	4:I:2:LEU:C	2.08	0.79
2:B:1083:ASP:OD2	2:B:1085:ALA:HB3	1.82	0.79
2:B:1097:ALA:HB2	2:B:1330:ILE:HG21	1.63	0.78
2:B:2185:PHE:HB3	2:B:2326:ASP:OD2	1.83	0.78
3:C:36:LYS:O	3:C:40:GLU:HG2	1.83	0.78
2:B:1151:ASN:HB3	2:B:1157:PHE:CD1	2.19	0.77
2:B:1116:LEU:HD21	2:B:1225:MET:CB	2.14	0.77
1:A:297:ILE:H	1:A:297:ILE:CD1	1.99	0.76
2:B:1290:GLY:O	2:B:1294:VAL:HG23	1.86	0.76
1:A:307:LEU:HB3	1:A:383:LEU:HD22	1.68	0.75
4:J:8:LEU:C	4:J:10:GLY:H	1.94	0.75
2:B:1044:LEU:HD13	2:B:1061:ILE:HD11	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2064:LEU:HB3	2:B:2111:LEU:CD2	2.17	0.75
1:A:283:SER:O	1:A:286:GLU:HB2	1.88	0.73
2:B:2229:ILE:HD13	2:B:2281:THR:HA	1.70	0.73
2:B:1129:THR:HG23	2:B:1132:GLU:OE1	1.88	0.73
1:A:217:ILE:HD11	1:A:264:ASN:ND2	2.03	0.73
2:B:1066:ASP:HA	2:B:1333:ASN:HA	1.70	0.73
2:B:2142:VAL:HG13	2:B:2178:ILE:HB	1.72	0.72
4:J:36:ILE:HG21	4:J:71:LEU:HD22	1.72	0.72
2:B:1012:ILE:O	2:B:1040:HIS:HA	1.90	0.72
4:J:27:LYS:HB3	4:J:38:PRO:HA	1.70	0.72
4:J:36:ILE:HB	4:J:41:GLN:NE2	2.05	0.72
4:J:3:ILE:HD11	4:J:17:ILE:HB	1.72	0.71
1:A:311:LEU:O	1:A:315:VAL:HG23	1.91	0.71
2:B:1049:PRO:HG3	2:B:1071:TYR:CE1	2.25	0.71
2:B:1117:ILE:HD11	2:B:1233:TRP:HE1	1.55	0.71
4:I:24:GLU:O	4:I:28:GLU:HG3	1.91	0.70
1:A:450:VAL:O	1:A:454:ILE:HG12	1.91	0.70
2:B:1296:LYS:HD3	2:B:1297:ASP:N	2.06	0.70
4:J:15:ILE:O	4:J:15:ILE:HG22	1.91	0.70
2:B:1122:LEU:HD12	2:B:1122:LEU:N	2.07	0.70
2:B:2237:TRP:HB3	2:B:2238:PRO:HD3	1.74	0.70
2:B:2052:LEU:HD11	2:B:2078:ILE:HG13	1.71	0.70
1:A:51:LEU:HD11	2:B:2092:PHE:HB3	1.74	0.69
1:A:268:ALA:O	1:A:272:VAL:HG23	1.92	0.69
1:A:419:PRO:HB2	1:A:475:LYS:HE3	1.74	0.69
1:A:358:GLY:O	1:A:361:VAL:HG22	1.92	0.69
4:J:8:LEU:O	4:J:10:GLY:N	2.25	0.69
2:B:1155:PRO:HD3	2:B:1345:ARG:HG3	1.73	0.69
4:I:50:MET:HE1	4:I:61:ILE:HD11	1.74	0.69
4:J:25:ARG:HA	4:J:28:GLU:CD	2.16	0.69
1:A:517:ASN:O	1:A:518:ASN:HB2	1.92	0.69
1:A:261:ASP:HB3	4:J:74:ARG:HH21	1.57	0.69
1:A:261:ASP:CB	4:J:74:ARG:NH2	2.56	0.69
4:J:36:ILE:HG22	4:J:41:GLN:HE21	1.58	0.69
3:C:43:LEU:HD11	3:C:49:ILE:HG22	1.75	0.68
4:J:2:LEU:N	4:J:2:LEU:HD12	2.07	0.68
4:J:56:ALA:O	4:J:61:ILE:HD12	1.94	0.67
2:B:2403:ARG:NH1	3:C:54:PRO:HD3	2.09	0.67
2:B:1151:ASN:HB3	2:B:1157:PHE:HD1	1.56	0.67
2:B:1185:ASP:HB2	2:B:1366:GLN:HB2	1.76	0.67
4:J:36:ILE:CG2	4:J:41:GLN:HE21	2.06	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1048:PHE:HE1	2:B:1058:PRO:HG2	1.59	0.67
1:A:60:ILE:HD12	1:A:60:ILE:N	2.10	0.67
4:I:39:GLN:CD	4:I:39:GLN:H	1.99	0.67
1:A:368:ILE:HG22	1:A:370:GLN:HG2	1.76	0.67
2:B:1123:LEU:HD11	2:B:1125:ASN:HB2	1.76	0.66
2:B:1118:TYR:CZ	2:B:1126:PRO:HG3	2.30	0.66
2:B:1292:GLU:HG3	2:B:1293:ALA:N	2.08	0.66
4:J:17:ILE:HG23	4:J:18:GLU:O	1.96	0.66
1:A:297:ILE:HD13	1:A:297:ILE:N	2.08	0.66
1:A:397:SER:OG	1:A:400:GLU:HG3	1.95	0.66
1:A:335:ASP:OD1	1:A:338:LYS:HD3	1.96	0.66
2:B:1048:PHE:HB3	2:B:1049:PRO:HD3	1.78	0.65
2:B:1240:LYS:O	2:B:1240:LYS:HG2	1.95	0.65
4:I:39:GLN:OE1	4:I:39:GLN:N	2.29	0.65
2:B:2216:CYS:SG	4:J:75:GLY:O	2.54	0.65
1:A:298:THR:HG23	1:A:301:THR:H	1.61	0.65
4:J:30:VAL:O	4:J:34:GLU:HB2	1.97	0.65
2:B:1127:PRO:HD3	2:B:1225:MET:HE1	1.78	0.65
2:B:1119:ASN:OD1	2:B:1122:LEU:HD13	1.97	0.65
1:A:281:ILE:HD12	1:A:323:LEU:HG	1.78	0.64
2:B:1073:GLN:HE22	2:B:1335:PRO:HG2	1.62	0.64
3:C:120:LYS:H	3:C:123:LEU:HD12	1.61	0.64
2:B:1116:LEU:HD21	2:B:1225:MET:HB3	1.78	0.64
2:B:2016:ARG:NH2	2:B:2116:PRO:HG2	2.11	0.64
1:A:310:ALA:HB2	1:A:361:VAL:HG12	1.78	0.64
2:B:1116:LEU:HD23	2:B:1116:LEU:C	2.22	0.64
1:A:133:GLU:O	1:A:137:LEU:HD12	1.98	0.64
2:B:1065:HIS:NE2	2:B:1331:MET:O	2.30	0.64
4:J:36:ILE:CB	4:J:41:GLN:HE21	2.10	0.64
2:B:2050:LYS:H	2:B:2139:HIS:HD2	1.44	0.64
4:J:15:ILE:HG23	4:J:29:ARG:CD	2.16	0.64
3:C:165:GLN:O	3:C:169:ARG:HG3	1.97	0.63
2:B:1116:LEU:HB2	2:B:1248:LEU:HD23	1.80	0.63
2:B:2183:GLU:HG3	4:I:73:LEU:HB3	1.79	0.63
4:I:37:PRO:HB3	4:I:39:GLN:NE2	2.13	0.63
2:B:2357:PRO:HD2	2:B:2442:SER:HB2	1.81	0.63
2:B:1127:PRO:CD	2:B:1225:MET:HE1	2.29	0.63
1:A:213:PRO:HB2	1:A:216:VAL:HG23	1.81	0.62
2:B:1010:ILE:HG12	2:B:1060:ILE:CG2	2.29	0.62
2:B:1025:GLY:HA2	2:B:1280:PHE:HE2	1.63	0.62
2:B:1060:ILE:HD11	2:B:1265:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1216:ALA:O	2:B:1220:LYS:HD2	1.98	0.62
2:B:2267:ARG:HG2	2:B:2267:ARG:HH11	1.63	0.62
2:B:1107:TYR:HD1	2:B:1281:LEU:HD13	1.64	0.62
4:I:70:VAL:CG1	4:I:71:LEU:N	2.63	0.62
1:A:154:ARG:HG3	1:A:154:ARG:HH11	1.64	0.62
1:A:8:LEU:HA	1:A:11:GLN:NE2	2.14	0.62
1:A:365:LEU:CD1	1:A:372:PRO:HA	2.29	0.62
4:J:75:GLY:O	4:J:76:GLY:C	2.41	0.62
3:C:130:TYR:CE1	4:J:11:LYS:HB2	2.35	0.61
1:A:373:GLU:O	1:A:373:GLU:HG2	2.01	0.61
2:B:1063:TRP:HB3	2:B:1068:PHE:HE1	1.65	0.61
2:B:1273:ASN:HB3	2:B:1276:LEU:HD12	1.82	0.61
2:B:1061:ILE:O	2:B:1265:ALA:HA	2.00	0.61
2:B:1337:MET:O	2:B:1340:PHE:HB3	2.01	0.61
2:B:2381:ILE:HG22	2:B:2392:LEU:HD12	1.81	0.61
2:B:1171:LYS:HD2	2:B:1181:ASP:OD2	2.00	0.61
1:A:481:GLU:OE1	1:A:484:ARG:HD3	2.00	0.61
1:A:516:PHE:H	1:A:516:PHE:HD2	1.47	0.61
2:B:1110:ALA:CB	2:B:1263:LEU:HD23	2.30	0.61
4:J:17:ILE:CD1	4:J:26:ILE:HG12	2.31	0.61
2:B:1068:PHE:HD1	2:B:1068:PHE:H	1.48	0.61
4:J:6:LYS:HD3	4:J:68:HIS:CE1	2.36	0.61
3:C:160:PHE:O	3:C:164:VAL:HG23	2.01	0.60
1:A:421:ASN:O	1:A:424:VAL:HG12	2.01	0.60
1:A:409:LYS:O	1:A:413:ILE:HG13	2.01	0.60
1:A:281:ILE:CD1	1:A:323:LEU:HG	2.30	0.60
4:I:8:LEU:HD11	4:I:71:LEU:HB2	1.84	0.60
2:B:1155:PRO:HG2	2:B:1341:TRP:CE3	2.37	0.60
2:B:2134:PHE:O	2:B:2137:GLN:HG2	2.01	0.60
2:B:1043:LYS:HB2	2:B:1047:LYS:HE2	1.82	0.60
4:J:31:GLU:O	4:J:35:GLY:CA	2.49	0.60
1:A:201:LEU:HA	1:A:204:MET:HE2	1.84	0.59
1:A:422:GLU:CD	1:A:422:GLU:H	2.10	0.59
1:A:521:ILE:HD12	1:A:532:PHE:CE1	2.37	0.59
2:B:1021:LEU:HD13	2:B:1294:VAL:HG11	1.84	0.59
1:A:339:TYR:CD2	2:B:2223:ARG:HB2	2.37	0.59
2:B:2149:ILE:HG23	3:C:88:HIS:HB3	1.84	0.59
2:B:2389:ASN:OD1	3:C:31:GLN:HG2	2.03	0.59
1:A:299:LYS:HA	1:A:368:ILE:HG23	1.84	0.59
2:B:2046:LEU:HD22	2:B:2073:ARG:CZ	2.33	0.59
1:A:353:ASP:O	1:A:357:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:HG2	1:A:197:GLN:NE2	2.17	0.59
2:B:1109:ILE:HG12	2:B:1264:SER:HA	1.85	0.59
2:B:1122:LEU:HD12	2:B:1122:LEU:H	1.68	0.59
2:B:1159:TRP:N	2:B:1160:PRO:HD2	2.18	0.59
1:A:236:THR:HB	1:A:239:GLU:HG3	1.85	0.58
4:J:61:ILE:HG23	4:J:65:SER:OG	2.03	0.58
1:A:209:HIS:CE1	1:A:252:LEU:HG	2.39	0.58
2:B:1021:LEU:HB2	2:B:1294:VAL:HG13	1.86	0.58
2:B:1149:MET:HB2	2:B:1223:THR:HG21	1.85	0.58
2:B:1197:VAL:O	2:B:1200:ILE:HB	2.03	0.58
4:J:6:LYS:HA	4:J:12:GLU:HA	1.85	0.58
1:A:59:ILE:C	1:A:60:ILE:HD12	2.28	0.58
3:C:163:ASN:HB3	3:C:173:ILE:HD12	1.86	0.58
1:A:184:ARG:NH1	1:A:325:VAL:HG22	2.18	0.58
3:C:21:LYS:O	3:C:23:SER:N	2.37	0.58
4:J:36:ILE:O	4:J:41:GLN:NE2	2.37	0.58
2:B:2407:ASN:HA	2:B:2410:LYS:HD2	1.84	0.57
4:J:43:LEU:HD21	4:J:69:LEU:HD13	1.86	0.57
2:B:1080:ILE:HD12	2:B:1107:TYR:CE2	2.38	0.57
2:B:1118:TYR:HB3	2:B:1225:MET:HE2	1.86	0.57
2:B:2213:PHE:CD1	2:B:2230:GLU:HG3	2.38	0.57
2:B:1123:LEU:CD1	2:B:1125:ASN:HB2	2.34	0.57
3:C:146:ASN:C	3:C:146:ASN:HD22	2.11	0.57
2:B:2401:GLU:HG3	2:B:2402:GLU:N	2.19	0.57
1:A:36:ILE:O	1:A:37:ASN:HB2	2.04	0.57
2:B:1145:LYS:HB3	2:B:1222:GLU:O	2.04	0.57
4:J:44:ILE:HA	4:J:49:GLN:HA	1.86	0.56
2:B:1010:ILE:HG23	2:B:1060:ILE:HG23	1.86	0.56
2:B:1068:PHE:HA	2:B:1071:TYR:CD2	2.39	0.56
1:A:309:ARG:HG3	1:A:364:LEU:HD11	1.87	0.56
1:A:461:LEU:O	1:A:465:LEU:HG	2.03	0.56
2:B:1116:LEU:HD23	2:B:1117:ILE:N	2.20	0.56
2:B:1140:LEU:CD1	2:B:1147:ALA:HA	2.34	0.56
2:B:1163:ALA:HA	2:B:1167:GLY:HA3	1.88	0.56
2:B:1216:ALA:O	2:B:1220:LYS:CD	2.53	0.56
2:B:2116:PRO:O	2:B:2117:ASN:HB2	2.05	0.56
1:A:12:LYS:O	2:B:2089:ASN:HB3	2.06	0.56
2:B:2376:MET:HB3	2:B:2427:ASP:OD2	2.05	0.56
2:B:1004:GLU:OE1	2:B:1004:GLU:HA	2.05	0.56
2:B:1150:PHE:CE1	2:B:1205:MET:HE1	2.40	0.56
2:B:2286:LYS:HB2	2:B:2288:ILE:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1021:LEU:HD13	2:B:1294:VAL:CG1	2.35	0.56
2:B:1280:PHE:HA	2:B:1284:TYR:HB2	1.88	0.56
2:B:2178:ILE:HD12	2:B:2191:VAL:HG22	1.88	0.56
4:J:8:LEU:C	4:J:10:GLY:N	2.56	0.56
2:B:1118:TYR:CB	2:B:1225:MET:HE2	2.37	0.55
2:B:2032:HIS:HB3	2:B:2313:SER:O	2.06	0.55
1:A:218:ILE:O	1:A:222:LEU:HB2	2.06	0.55
1:A:265:PHE:O	1:A:269:ILE:HG12	2.05	0.55
1:A:517:ASN:O	1:A:517:ASN:OD1	2.25	0.55
2:B:1243:TYR:CD2	2:B:1243:TYR:N	2.75	0.55
1:A:217:ILE:HD11	1:A:264:ASN:HD22	1.70	0.55
2:B:1020:GLY:HA2	2:B:1023:GLU:OE2	2.06	0.55
2:B:1011:TRP:HB3	2:B:1044:LEU:HD22	1.89	0.55
2:B:1090:LEU:HD23	2:B:1305:LEU:HA	1.89	0.55
2:B:1236:ILE:HG21	2:B:1243:TYR:CD1	2.41	0.55
2:B:2081:ASP:HB3	2:B:2103:LYS:HE3	1.87	0.55
2:B:1288:ASP:O	2:B:1292:GLU:HG2	2.07	0.55
1:A:307:LEU:HD22	1:A:383:LEU:HD22	1.87	0.55
1:A:309:ARG:CG	1:A:364:LEU:HD11	2.37	0.55
2:B:2040:GLU:OE1	2:B:2040:GLU:HA	2.07	0.55
2:B:2223:ARG:H	2:B:2227:HIS:HD2	1.53	0.55
2:B:1097:ALA:HB2	2:B:1330:ILE:CG2	2.35	0.55
3:C:41:LEU:HD23	3:C:42:ASN:H	1.72	0.55
2:B:2015:GLY:HA2	2:B:2018:ASN:OD1	2.07	0.55
2:B:1151:ASN:HB2	2:B:1211:TYR:HA	1.89	0.54
2:B:1155:PRO:O	2:B:1159:TRP:HB2	2.06	0.54
2:B:2245:GLU:HG3	3:C:147:LYS:CD	2.37	0.54
1:A:351:LYS:O	1:A:354:ALA:HB3	2.08	0.54
4:I:35:GLY:O	4:I:37:PRO:HD3	2.08	0.54
3:C:8:LYS:HB3	3:C:10:GLN:HE21	1.72	0.54
2:B:1068:PHE:CD1	2:B:1068:PHE:N	2.74	0.54
4:I:2:LEU:C	4:I:2:LEU:CD1	2.80	0.54
4:J:34:GLU:OE1	4:J:34:GLU:HA	2.06	0.54
2:B:1220:LYS:HB2	2:B:1222:GLU:HG3	1.90	0.54
3:C:72:LYS:O	3:C:73:SER:HB2	2.07	0.54
4:J:17:ILE:HG23	4:J:18:GLU:N	2.23	0.54
4:J:3:ILE:CD1	4:J:17:ILE:HB	2.38	0.54
2:B:1161:LEU:HD21	2:B:1195:PHE:HD2	1.71	0.53
2:B:2245:GLU:HG3	3:C:147:LYS:HD3	1.90	0.53
1:A:61:ASP:HB3	1:A:86:ALA:HB2	1.90	0.53
1:A:367:SER:C	1:A:368:ILE:HD12	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1013:ASN:ND2	2:B:1015:ASP:OD1	2.41	0.53
4:J:59:TYR:HB2	4:J:61:ILE:HD11	1.89	0.53
1:A:15:ARG:NH1	7:B:103:ATP:O2G	2.41	0.53
2:B:1116:LEU:HD21	2:B:1225:MET:HB2	1.89	0.53
2:B:2411:THR:OG1	2:B:2414:GLU:HG3	2.08	0.53
2:B:1080:ILE:HG22	2:B:1267:ILE:HD12	1.89	0.53
4:J:45:TYR:O	4:J:46:SER:HB3	2.07	0.53
2:B:1116:LEU:HD11	2:B:1225:MET:SD	2.49	0.53
1:A:323:LEU:HB3	1:A:324:PRO:HD2	1.89	0.53
4:J:44:ILE:HG12	4:J:49:GLN:HB3	1.90	0.53
1:A:313:GLU:OE2	1:A:313:GLU:HA	2.09	0.53
1:A:396:ARG:NH1	1:A:408:ASN:HB2	2.20	0.53
2:B:1080:ILE:HD11	2:B:1104:LEU:HB3	1.91	0.53
4:I:70:VAL:HG12	4:I:71:LEU:N	2.24	0.53
1:A:518:ASN:CG	1:A:534:LEU:H	2.18	0.52
4:J:36:ILE:C	4:J:41:GLN:NE2	2.68	0.52
1:A:54:ILE:O	1:A:100:VAL:HG22	2.10	0.52
1:A:90:MET:HE2	1:A:104:PHE:HD2	1.74	0.52
2:B:1025:GLY:HA2	2:B:1280:PHE:CE2	2.44	0.52
3:C:139:PRO:HB2	3:C:153:LEU:CD2	2.39	0.52
1:A:189:PHE:CE2	1:A:192:LEU:HD22	2.44	0.52
2:B:1122:LEU:H	2:B:1122:LEU:CD1	2.22	0.52
4:J:54:LYS:HD2	4:J:59:TYR:OH	2.09	0.52
1:A:154:ARG:HG3	1:A:154:ARG:NH1	2.25	0.52
2:B:1139:GLU:O	2:B:1142:ALA:HB3	2.10	0.52
2:B:2025:GLU:O	2:B:2037:PRO:HB3	2.10	0.52
2:B:1073:GLN:HG2	2:B:2119:ASN:ND2	2.24	0.52
2:B:1119:ASN:CG	2:B:1122:LEU:HD13	2.34	0.52
3:C:164:VAL:HG12	3:C:168:MET:HE2	1.92	0.52
1:A:34:CYS:SG	1:A:60:ILE:HD13	2.51	0.51
2:B:2182:THR:O	4:I:75:GLY:HA3	2.10	0.51
2:B:2231:TYR:CD2	2:B:2267:ARG:HD3	2.45	0.51
1:A:521:ILE:HD12	1:A:532:PHE:HE1	1.75	0.51
2:B:1122:LEU:N	2:B:1122:LEU:CD1	2.74	0.51
2:B:1140:LEU:O	2:B:1144:GLY:N	2.43	0.51
1:A:46:LEU:HD21	1:A:57:PHE:CD1	2.46	0.51
2:B:1220:LYS:HE2	2:B:1222:GLU:OE2	2.11	0.51
2:B:2017:TRP:O	2:B:2021:LYS:HG3	2.09	0.51
1:A:298:THR:HG23	1:A:301:THR:N	2.26	0.51
2:B:2370:ASN:O	2:B:2371:SER:C	2.54	0.51
1:A:65:VAL:HB	1:A:80:SER:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:TYR:HA	3:C:168:MET:HE1	1.92	0.51
2:B:1215:GLU:HG2	2:B:1219:ASN:ND2	2.14	0.51
2:B:2369:THR:HG22	2:B:2376:MET:O	2.11	0.51
4:J:45:TYR:O	4:J:45:TYR:CG	2.64	0.51
4:J:36:ILE:HB	4:J:41:GLN:HE21	1.70	0.51
2:B:1296:LYS:HD3	2:B:1296:LYS:C	2.37	0.50
2:B:2050:LYS:H	2:B:2139:HIS:CD2	2.27	0.50
2:B:2081:ASP:HB2	7:B:103:ATP:O2'	2.11	0.50
1:A:200:ASP:O	1:A:204:MET:HG3	2.11	0.50
1:A:405:ASP:OD1	1:A:405:ASP:N	2.43	0.50
2:B:2224:LEU:H	2:B:2227:HIS:CD2	2.29	0.50
1:A:311:LEU:HD11	1:A:383:LEU:CD1	2.33	0.50
2:B:1190:LYS:HG2	2:B:1362:LEU:HD12	1.93	0.50
2:B:2380:ALA:O	2:B:2425:VAL:HA	2.11	0.50
1:A:90:MET:HE2	1:A:104:PHE:CD2	2.46	0.50
4:J:5:VAL:HG22	4:J:13:ILE:CG2	2.29	0.50
1:A:287:ASP:O	1:A:291:ASP:HB2	2.11	0.50
1:A:422:GLU:HG3	1:A:530:ALA:HB3	1.94	0.50
2:B:1107:TYR:CD1	2:B:1281:LEU:HD13	2.46	0.50
4:I:53:GLU:OE2	4:I:53:GLU:HA	2.12	0.50
2:B:1133:ILE:N	2:B:1134:PRO:HD2	2.27	0.50
2:B:2420:GLY:O	2:B:2437:LYS:HG3	2.12	0.50
3:C:56:ASP:CG	3:C:59:ASN:HD22	2.19	0.50
2:B:1078:ALA:HB2	2:B:1274:LYS:HE3	1.93	0.50
2:B:2375:GLN:HG3	2:B:2375:GLN:O	2.12	0.50
1:A:128:ALA:HB1	1:A:131:LEU:HD11	1.94	0.49
2:B:1196:LEU:O	2:B:1200:ILE:HG12	2.12	0.49
1:A:190:PRO:O	1:A:194:GLU:HG3	2.12	0.49
1:A:215:ILE:CD1	1:A:332:MET:HE1	2.43	0.49
2:B:1132:GLU:C	2:B:1134:PRO:HD2	2.37	0.49
1:A:77:GLN:NE2	1:A:77:GLN:HA	2.28	0.49
1:A:335:ASP:CG	1:A:338:LYS:HD3	2.37	0.49
1:A:365:LEU:HD13	1:A:371:ALA:O	2.13	0.49
1:A:473:MET:HE3	1:A:473:MET:O	2.12	0.49
2:B:1017:GLY:N	2:B:1298:LYS:HD2	2.28	0.49
3:C:21:LYS:C	3:C:23:SER:H	2.21	0.49
4:I:55:THR:HG22	4:I:58:ASP:CG	2.38	0.49
4:J:15:ILE:O	4:J:16:ASP:C	2.55	0.49
1:A:33:VAL:HG12	1:A:54:ILE:HD13	1.94	0.49
2:B:1155:PRO:HG2	2:B:1341:TRP:HE3	1.78	0.49
2:B:1258:PRO:HG3	2:B:1324:ASN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:HIS:HA	1:A:441:ARG:O	2.12	0.49
2:B:1151:ASN:HB2	2:B:1211:TYR:CA	2.43	0.49
2:B:1116:LEU:HD21	2:B:1225:MET:SD	2.53	0.49
4:J:74:ARG:HG3	4:J:75:GLY:H	1.77	0.49
2:B:1336:GLN:NE2	2:B:1339:ALA:HB3	2.27	0.49
1:A:77:GLN:HA	1:A:77:GLN:HE21	1.77	0.48
1:A:121:CYS:HA	1:A:148:ILE:HD11	1.95	0.48
1:A:262:GLU:C	1:A:264:ASN:N	2.71	0.48
2:B:1020:GLY:N	2:B:1297:ASP:OD2	2.41	0.48
2:B:1158:THR:C	2:B:1160:PRO:HD2	2.38	0.48
1:A:137:LEU:HD11	1:A:402:TYR:CD2	2.48	0.48
2:B:1118:TYR:HA	2:B:1224:ALA:O	2.13	0.48
2:B:1152:LEU:HD13	2:B:1207:ALA:HA	1.95	0.48
1:A:229:THR:OG1	1:A:232:ARG:HB2	2.13	0.48
2:B:2278:TYR:O	2:B:2282:GLN:HG3	2.13	0.48
4:J:31:GLU:HA	4:J:36:ILE:N	2.28	0.48
1:A:60:ILE:N	1:A:60:ILE:CD1	2.75	0.48
2:B:1029:GLU:HB3	2:B:1035:LYS:HA	1.95	0.48
4:J:15:ILE:HD13	4:J:29:ARG:HB2	1.96	0.48
2:B:1011:TRP:CD1	2:B:1058:PRO:HB3	2.49	0.48
2:B:1159:TRP:N	2:B:1160:PRO:CD	2.77	0.48
2:B:2032:HIS:HD2	2:B:2034:ASP:H	1.60	0.48
1:A:504:GLU:HG3	1:A:516:PHE:CE2	2.49	0.48
3:C:169:ARG:HH11	3:C:169:ARG:HG2	1.77	0.48
2:B:1336:GLN:HE21	2:B:1339:ALA:HB3	1.78	0.48
1:A:68:GLU:HG2	2:B:2018:ASN:HB2	1.96	0.48
2:B:1271:SER:O	2:B:1274:LYS:HG3	2.13	0.48
2:B:1044:LEU:HD12	2:B:1045:GLU:N	2.29	0.48
2:B:1082:PRO:HB3	2:B:1282:GLU:OE2	2.14	0.47
2:B:1243:TYR:N	2:B:1243:TYR:HD2	2.11	0.47
1:A:49:LEU:O	1:A:52:PRO:HG2	2.15	0.47
4:J:5:VAL:O	4:J:5:VAL:CG2	2.62	0.47
1:A:422:GLU:O	1:A:425:LEU:HB2	2.15	0.47
2:B:2179:ASP:OD1	2:B:2190:ARG:NH1	2.47	0.47
4:I:5:VAL:HA	4:I:67:LEU:O	2.14	0.47
1:A:220:LYS:O	1:A:223:ALA:N	2.41	0.47
1:A:121:CYS:HA	1:A:148:ILE:CD1	2.45	0.47
1:A:311:LEU:CD1	1:A:383:LEU:HD11	2.37	0.47
2:B:2032:HIS:CD2	2:B:2034:ASP:H	2.33	0.47
2:B:2152:ARG:NE	2:B:2201:GLU:OE2	2.47	0.47
2:B:1073:GLN:NE2	2:B:1335:PRO:HG2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1145:LYS:N	2:B:1145:LYS:HD2	2.30	0.47
3:C:71:TYR:HA	3:C:168:MET:CE	2.45	0.47
2:B:1071:TYR:HB3	2:B:1076:LEU:HB2	1.97	0.47
2:B:2318:LEU:HD11	2:B:2334:THR:HG23	1.97	0.47
3:C:132:LEU:O	3:C:135:LEU:HB2	2.15	0.47
2:B:1126:PRO:CB	2:B:1246:THR:OG1	2.63	0.47
2:B:1344:VAL:HA	2:B:1347:ALA:HB3	1.97	0.47
1:A:261:ASP:CB	4:J:74:ARG:HH22	2.26	0.46
1:A:371:ALA:C	1:A:373:GLU:H	2.23	0.46
2:B:1126:PRO:HB3	2:B:1246:THR:OG1	2.14	0.46
2:B:1131:GLU:N	2:B:1131:GLU:OE1	2.48	0.46
4:I:71:LEU:HD12	4:I:71:LEU:HA	1.78	0.46
2:B:1123:LEU:HG	2:B:1125:ASN:O	2.15	0.46
3:C:112:LEU:O	3:C:116:ARG:HG2	2.15	0.46
2:B:1077:LEU:HD12	2:B:1105:ILE:HD12	1.96	0.46
2:B:1345:ARG:O	2:B:1349:ILE:HG12	2.15	0.46
2:B:2026:ARG:O	2:B:2037:PRO:HG3	2.14	0.46
2:B:1111:VAL:HG12	2:B:1112:GLU:N	2.31	0.46
2:B:1151:ASN:HD21	2:B:1154:GLU:HG2	1.80	0.46
2:B:2217:THR:HG23	2:B:2223:ARG:NH2	2.30	0.46
1:A:191:GLU:H	1:A:191:GLU:CD	2.21	0.46
1:A:484:ARG:HH11	2:B:2027:SER:C	2.23	0.46
2:B:2058:GLY:N	2:B:2091:GLN:HG2	2.29	0.46
4:J:36:ILE:CB	4:J:41:GLN:NE2	2.71	0.46
2:B:1086:PHE:CD1	2:B:1086:PHE:C	2.92	0.46
1:A:496:PHE:C	1:A:496:PHE:CD2	2.94	0.46
2:B:1047:LYS:HD3	2:B:1047:LYS:N	2.31	0.46
4:I:70:VAL:HG13	4:I:71:LEU:H	1.80	0.46
1:A:15:ARG:HH12	7:B:103:ATP:PG	2.38	0.46
2:B:1118:TYR:HD1	2:B:1118:TYR:H	1.64	0.46
2:B:1130:TRP:HD1	2:B:1250:THR:O	1.99	0.46
3:C:44:PRO:HG3	3:C:130:TYR:HE2	1.81	0.46
1:A:116:ASP:HB3	1:A:119:PHE:HB2	1.98	0.46
2:B:1080:ILE:HD12	2:B:1107:TYR:CD2	2.51	0.46
4:I:70:VAL:CG1	4:I:71:LEU:H	2.29	0.46
1:A:337:GLY:O	1:A:341:LYS:HB2	2.15	0.46
1:A:430:ARG:NH1	1:A:464:PHE:CE1	2.84	0.46
2:B:1114:LEU:O	2:B:1248:LEU:HD11	2.16	0.46
1:A:15:ARG:NH1	7:B:103:ATP:PG	2.89	0.45
4:J:4:LYS:CG	4:J:14:GLU:HG2	2.46	0.45
2:B:1118:TYR:CE1	2:B:1246:THR:HB	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1208:ASP:OD2	2:B:1208:ASP:N	2.46	0.45
1:A:33:VAL:CG1	1:A:54:ILE:HD13	2.47	0.45
1:A:87:GLU:O	1:A:91:GLU:HG3	2.17	0.45
1:A:254:ASN:HB3	1:A:260:GLU:OE2	2.16	0.45
1:A:516:PHE:CD2	1:A:516:PHE:N	2.85	0.45
2:B:2187:GLY:CA	4:I:73:LEU:HD13	2.46	0.45
1:A:458:LYS:O	1:A:458:LYS:HD3	2.16	0.45
1:A:489:GLU:H	2:B:2019:HIS:CE1	2.34	0.45
2:B:1064:ALA:HA	2:B:1262:VAL:O	2.17	0.45
3:C:94:LYS:HE3	3:C:107:GLU:O	2.17	0.45
2:B:1020:GLY:C	2:B:1023:GLU:HG2	2.42	0.45
4:J:29:ARG:C	4:J:31:GLU:N	2.68	0.45
2:B:1149:MET:CB	2:B:1223:THR:HG21	2.46	0.45
2:B:2405:ARG:N	2:B:2406:PRO:CD	2.80	0.45
4:J:59:TYR:O	4:J:60:LYS:C	2.60	0.45
1:A:317:LYS:HB3	1:A:318:GLU:OE2	2.16	0.45
3:C:38:ILE:O	3:C:41:LEU:HB2	2.17	0.45
2:B:1137:ASP:OD1	2:B:1141:LYS:NZ	2.45	0.45
2:B:2252:ASP:O	2:B:2254:PRO:HD3	2.17	0.45
4:I:5:VAL:HG13	4:I:13:ILE:HG12	1.99	0.45
1:A:227:SER:C	1:A:229:THR:H	2.25	0.45
1:A:233:ILE:O	1:A:234:PRO:C	2.60	0.45
2:B:1095:TRP:HA	2:B:1098:VAL:CG2	2.46	0.45
2:B:2170:ASP:C	2:B:2170:ASP:OD2	2.59	0.45
2:B:2233:ARG:NH2	3:C:117:GLU:OE2	2.50	0.45
1:A:310:ALA:CB	1:A:361:VAL:HG12	2.44	0.44
4:J:5:VAL:HA	4:J:67:LEU:HB2	1.98	0.44
1:A:262:GLU:C	1:A:264:ASN:H	2.24	0.44
2:B:1129:THR:HG23	2:B:1132:GLU:CD	2.42	0.44
2:B:2110:PHE:C	2:B:2110:PHE:CD2	2.96	0.44
3:C:67:ASP:HA	3:C:72:LYS:HG3	2.00	0.44
3:C:146:ASN:C	3:C:146:ASN:ND2	2.75	0.44
4:I:45:TYR:CB	4:I:50:MET:HE3	2.48	0.44
2:B:1006:GLY:O	2:B:1034:ILE:HD12	2.17	0.44
2:B:1218:PHE:CD2	2:B:1226:THR:HG22	2.53	0.44
4:J:13:ILE:HG23	4:J:13:ILE:O	2.17	0.44
2:B:1065:HIS:HB2	2:B:1097:ALA:O	2.18	0.44
2:B:1275:GLU:HA	2:B:1275:GLU:OE1	2.18	0.44
2:B:2155:ASN:HB2	2:B:2200:ILE:HG13	1.99	0.44
1:A:33:VAL:O	1:A:57:PHE:HA	2.18	0.44
1:A:255:GLU:H	1:A:255:GLU:HG3	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1163:ALA:HA	2:B:1167:GLY:CA	2.47	0.44
2:B:2267:ARG:HH11	2:B:2267:ARG:CG	2.29	0.44
4:J:27:LYS:HB3	4:J:41:GLN:OE1	2.17	0.44
3:C:105:ASP:OD1	3:C:109:ASN:N	2.51	0.44
4:J:6:LYS:HB3	4:J:68:HIS:ND1	2.33	0.44
2:B:1086:PHE:HA	2:B:1089:LYS:HE3	2.00	0.44
2:B:1100:TYR:CE2	2:B:1101:ASN:OD1	2.71	0.44
2:B:1177:TYR:HE1	2:B:1332:PRO:HA	1.82	0.44
2:B:1251:PHE:O	2:B:1252:LYS:C	2.61	0.44
2:B:1323:GLU:HG2	2:B:1327:LYS:HE3	1.98	0.44
2:B:2224:LEU:O	2:B:2227:HIS:HB2	2.18	0.44
4:J:7:THR:N	4:J:11:LYS:O	2.36	0.44
2:B:1063:TRP:HB3	2:B:1068:PHE:CE1	2.50	0.43
2:B:1228:ASN:HB3	2:B:1229:GLY:H	1.65	0.43
4:J:15:ILE:HG23	4:J:29:ARG:HH11	1.83	0.43
1:A:71:GLY:O	2:B:2069:LEU:HD22	2.18	0.43
1:A:401:GLU:HG3	1:A:534:LEU:OXT	2.18	0.43
3:C:42:ASN:HD22	3:C:42:ASN:C	2.26	0.43
2:B:2347:SER:OG	2:B:2348:GLN:NE2	2.51	0.43
2:B:2357:PRO:CD	2:B:2442:SER:HB2	2.48	0.43
4:J:1:MET:C	4:J:2:LEU:HD12	2.44	0.43
1:A:158:LEU:HD22	1:A:493:ILE:HD11	2.00	0.43
1:A:428:MET:HE2	1:A:479:VAL:HA	2.01	0.43
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.86	0.43
2:B:2062:GLU:HB3	2:B:2300:ALA:CB	2.49	0.43
4:J:27:LYS:O	4:J:31:GLU:HB3	2.18	0.43
1:A:110:GLU:HA	1:A:110:GLU:OE2	2.18	0.43
2:B:2113:ASP:OD1	2:B:2113:ASP:C	2.61	0.43
4:J:27:LYS:HB3	4:J:38:PRO:CA	2.45	0.43
1:A:364:LEU:HA	1:A:367:SER:OG	2.17	0.43
2:B:1052:ALA:C	2:B:1076:LEU:HD22	2.43	0.43
2:B:1093:PHE:HD1	2:B:1093:PHE:H	1.67	0.43
2:B:1230:PRO:HA	2:B:1233:TRP:CE3	2.53	0.43
2:B:2055:GLY:O	2:B:2060:GLY:HA3	2.18	0.43
1:A:15:ARG:NH1	7:B:103:ATP:O1G	2.50	0.43
2:B:1024:VAL:HG21	2:B:1294:VAL:CG2	2.49	0.43
2:B:2016:ARG:HH22	2:B:2116:PRO:HG2	1.81	0.43
4:I:8:LEU:HD23	4:I:8:LEU:HA	1.80	0.43
2:B:1068:PHE:HA	2:B:1071:TYR:HD2	1.81	0.43
4:I:4:LYS:HD3	4:I:12:GLU:CD	2.44	0.43
1:A:137:LEU:HA	1:A:398:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:O	1:A:246:LEU:HD12	2.18	0.43
1:A:439:GLN:C	1:A:441:ARG:H	2.27	0.43
2:B:1097:ALA:CB	2:B:1330:ILE:HG21	2.43	0.43
2:B:2128:GLN:H	2:B:2128:GLN:HG2	1.35	0.43
2:B:2142:VAL:CG1	2:B:2178:ILE:HB	2.46	0.43
2:B:2240:GLU:O	2:B:2241:GLN:C	2.62	0.43
1:A:184:ARG:NE	1:A:279:THR:HG21	2.34	0.43
2:B:1020:GLY:O	2:B:1023:GLU:HG2	2.18	0.43
3:C:3:LYS:HG2	3:C:4:LEU:N	2.33	0.43
2:B:1116:LEU:C	2:B:1116:LEU:CD2	2.90	0.42
1:A:368:ILE:CG2	1:A:370:GLN:HG2	2.48	0.42
2:B:1145:LYS:HB3	2:B:1145:LYS:HE3	1.79	0.42
2:B:1216:ALA:HA	2:B:1219:ASN:HD22	1.82	0.42
2:B:1323:GLU:O	2:B:1326:GLN:HB3	2.19	0.42
4:I:6:LYS:HG2	4:I:12:GLU:HB2	2.00	0.42
1:A:137:LEU:HD21	1:A:402:TYR:CG	2.54	0.42
1:A:220:LYS:O	1:A:221:TYR:C	2.62	0.42
1:A:488:ALA:HB2	2:B:2022:LYS:HG3	2.00	0.42
2:B:1117:ILE:HD11	2:B:1233:TRP:NE1	2.27	0.42
3:C:113:ASN:CG	3:C:114:ILE:H	2.28	0.42
1:A:128:ALA:HB1	1:A:131:LEU:CD1	2.49	0.42
1:A:446:SER:HB2	1:A:449:GLN:HG3	2.01	0.42
2:B:1148:LEU:HD12	2:B:1225:MET:O	2.18	0.42
2:B:1195:PHE:CZ	2:B:1199:LEU:HD11	2.54	0.42
2:B:2140:ILE:HG22	2:B:2141:ILE:N	2.35	0.42
2:B:2197:THR:O	2:B:2198:ALA:C	2.60	0.42
3:C:99:VAL:CG2	3:C:100:TYR:N	2.83	0.42
1:A:68:GLU:HG2	2:B:2018:ASN:CB	2.50	0.42
1:A:481:GLU:O	1:A:484:ARG:HB3	2.19	0.42
2:B:1060:ILE:HD11	2:B:1265:ALA:CB	2.48	0.42
2:B:2152:ARG:HE	2:B:2201:GLU:CD	2.27	0.42
2:B:1025:GLY:O	2:B:1028:PHE:HB3	2.20	0.42
2:B:1201:LYS:C	2:B:1203:LYS:H	2.27	0.42
4:J:27:LYS:HD3	4:J:38:PRO:O	2.19	0.42
1:A:367:SER:O	1:A:368:ILE:HD12	2.19	0.42
2:B:1098:VAL:O	2:B:1098:VAL:HG23	2.19	0.42
4:J:61:ILE:CG2	4:J:65:SER:OG	2.67	0.42
1:A:396:ARG:NH2	1:A:406:THR:O	2.52	0.42
1:A:517:ASN:O	1:A:518:ASN:CB	2.61	0.42
1:A:518:ASN:OD1	1:A:534:LEU:HB2	2.20	0.42
2:B:1063:TRP:CD1	2:B:1064:ALA:H	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1136:LEU:HD13	2:B:1139:GLU:OE1	2.20	0.42
2:B:1155:PRO:CB	2:B:1344:VAL:HG23	2.50	0.42
2:B:2041:SER:O	2:B:2044:PHE:HB3	2.19	0.42
4:J:6:LYS:HD3	4:J:68:HIS:ND1	2.32	0.42
1:A:105:VAL:O	1:A:105:VAL:CG2	2.68	0.42
2:B:1243:TYR:CD2	2:B:1243:TYR:C	2.98	0.42
2:B:1357:THR:O	2:B:1358:VAL:C	2.63	0.42
3:C:99:VAL:HG22	3:C:100:TYR:N	2.35	0.42
4:J:4:LYS:HG3	4:J:14:GLU:HG2	2.00	0.42
4:J:28:GLU:HA	4:J:31:GLU:OE1	2.19	0.42
2:B:1063:TRP:CD1	2:B:1067:ARG:HG3	2.55	0.41
2:B:1099:ARG:HG2	2:B:1100:TYR:N	2.34	0.41
1:A:19:LEU:HG	2:B:2290:PRO:HB3	2.02	0.41
1:A:187:LYS:N	1:A:188:PRO:HD3	2.34	0.41
1:A:201:LEU:HD11	1:A:220:LYS:HG3	2.02	0.41
2:B:1206:ASN:ND2	2:B:1208:ASP:OD1	2.54	0.41
2:B:1040:HIS:CD2	2:B:1040:HIS:N	2.87	0.41
2:B:1044:LEU:CD1	2:B:1061:ILE:HD11	2.46	0.41
3:C:72:LYS:O	3:C:73:SER:CB	2.68	0.41
4:I:2:LEU:HD12	4:I:3:ILE:N	2.35	0.41
1:A:58:THR:HA	1:A:103:SER:O	2.20	0.41
1:A:148:ILE:HA	1:A:149:PRO:HD3	1.74	0.41
1:A:293:ARG:HG2	1:A:305:TRP:CE2	2.55	0.41
2:B:1084:LYS:HA	2:B:1087:GLN:HE21	1.86	0.41
1:A:303:SER:O	1:A:304:PHE:C	2.64	0.41
2:B:1024:VAL:HG21	2:B:1294:VAL:HG22	2.02	0.41
2:B:1048:PHE:CE1	2:B:1058:PRO:HG2	2.48	0.41
2:B:2062:GLU:HG2	2:B:2300:ALA:HB3	2.03	0.41
2:B:1044:LEU:HA	2:B:1047:LYS:HB2	2.02	0.41
2:B:1147:ALA:O	2:B:1224:ALA:HB3	2.21	0.41
2:B:1163:ALA:O	2:B:1164:ALA:C	2.63	0.41
2:B:2126:LYS:O	2:B:2127:ILE:C	2.61	0.41
4:J:74:ARG:CG	4:J:75:GLY:H	2.33	0.41
1:A:216:VAL:O	1:A:217:ILE:C	2.64	0.41
1:A:507:LYS:HG2	1:A:513:PHE:HB2	2.03	0.41
2:B:1026:LYS:HB3	2:B:1026:LYS:HE2	1.93	0.41
2:B:1060:ILE:HG12	2:B:1061:ILE:N	2.36	0.41
4:J:31:GLU:C	4:J:35:GLY:H	2.29	0.41
4:J:40:GLN:C	4:J:41:GLN:HG3	2.46	0.41
1:A:435:PHE:CD2	1:A:443:PRO:HG3	2.56	0.41
4:I:2:LEU:HD12	4:I:2:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:15:ILE:CG2	4:J:15:ILE:O	2.62	0.41
4:J:43:LEU:CD2	4:J:69:LEU:HD13	2.51	0.41
4:J:66:VAL:O	4:J:67:LEU:HD23	2.21	0.41
1:A:9:LYS:HG3	1:A:13:TYR:CE1	2.56	0.40
2:B:1090:LEU:HD12	2:B:1095:TRP:CZ2	2.56	0.40
4:J:31:GLU:CB	4:J:36:ILE:O	2.52	0.40
1:A:355:ALA:O	1:A:356:ALA:C	2.65	0.40
2:B:1350:ASN:HB3	2:B:1356:GLN:HG2	2.02	0.40
2:B:2169:LEU:HD12	2:B:2170:ASP:N	2.36	0.40
4:I:4:LYS:HD3	4:I:12:GLU:OE2	2.21	0.40
2:B:1173:GLU:O	2:B:1174:ASN:C	2.64	0.40
2:B:2321:TYR:O	2:B:2334:THR:HA	2.22	0.40
2:B:2380:ALA:HB1	2:B:2394:LEU:CD1	2.52	0.40
4:J:37:PRO:O	4:J:41:GLN:HG3	2.21	0.40
2:B:1024:VAL:HG12	2:B:1024:VAL:O	2.20	0.40
2:B:1090:LEU:HA	2:B:1304:ALA:O	2.22	0.40
2:B:2411:THR:O	2:B:2414:GLU:N	2.55	0.40
1:A:6:LYS:C	1:A:8:LEU:H	2.29	0.40
1:A:56:SER:HB3	1:A:101:SER:HB2	2.04	0.40
2:B:1151:ASN:HB3	2:B:1157:PHE:CE1	2.56	0.40
2:B:1193:LEU:O	2:B:1197:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	528/536 (98%)	476 (90%)	49 (9%)	3 (1%)	21	51
2	B	783/805 (97%)	709 (90%)	62 (8%)	12 (2%)	8	28
3	C	174/180 (97%)	165 (95%)	8 (5%)	1 (1%)	21	51
4	I	74/81 (91%)	71 (96%)	2 (3%)	1 (1%)	9	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	J	74/81 (91%)	54 (73%)	17 (23%)	3 (4%)	2 8
All	All	1633/1683 (97%)	1475 (90%)	138 (8%)	20 (1%)	10 34

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	ASN
4	J	9	THR
4	J	46	SER
1	A	228	GLU
2	B	1017	GLY
2	B	1174	ASN
2	B	1209	THR
2	B	1351	ALA
3	C	22	GLY
4	I	63	GLY
2	B	2375	GLN
2	B	1082	PRO
2	B	1285	LEU
2	B	2049	CYS
4	J	16	ASP
1	A	190	PRO
2	B	1250	THR
2	B	2320	ASN
2	B	1166	GLY
2	B	1332	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	461/465 (99%)	443 (96%)	18 (4%)	28 64
2	B	663/675 (98%)	618 (93%)	45 (7%)	14 42
3	C	160/163 (98%)	151 (94%)	9 (6%)	19 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	66/68 (97%)	61 (92%)	5 (8%)	12	36
4	J	66/68 (97%)	58 (88%)	8 (12%)	5	16
All	All	1416/1439 (98%)	1331 (94%)	85 (6%)	17	47

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	83	LYS
1	A	105	VAL
1	A	154	ARG
1	A	171	VAL
1	A	190	PRO
1	A	245	ASP
1	A	277	ASN
1	A	297	ILE
1	A	347	ARG
1	A	405	ASP
1	A	422	GLU
1	A	430	ARG
1	A	439	GLN
1	A	471	SER
1	A	473	MET
1	A	503	GLN
1	A	516	PHE
2	B	1026	LYS
2	B	1031	ASP
2	B	1044	LEU
2	B	1045	GLU
2	B	1047	LYS
2	B	1068	PHE
2	B	1086	PHE
2	B	1118	TYR
2	B	1131	GLU
2	B	1145	LYS
2	B	1174	ASN
2	B	1208	ASP
2	B	1226	THR
2	B	1234	SER
2	B	1243	TYR
2	B	1259	PHE

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Mol	Chain	Res	Type
2	B	1263	LEU
2	B	1278	LYS
2	B	1292	GLU
2	B	1296	LYS
2	B	1359	ASP
2	B	2018	ASN
2	B	2074	GLN
2	B	2077	VAL
2	B	2078	ILE
2	B	2081	ASP
2	B	2082	THR
2	B	2114	ARG
2	B	2128	GLN
2	B	2142	VAL
2	B	2160	SER
2	B	2182	THR
2	B	2190	ARG
2	B	2210	GLN
2	B	2233	ARG
2	B	2241	GLN
2	B	2258	GLN
2	B	2262	GLN
2	B	2354	GLN
2	B	2362	GLN
2	B	2390	ARG
2	B	2395	GLN
2	B	2401	GLU
2	B	2425	VAL
2	B	2428	VAL
3	C	23	SER
3	C	41	LEU
3	C	42	ASN
3	C	52	SER
3	C	70	PHE
3	C	87	PRO
3	C	115	LEU
3	C	116	ARG
3	C	176	THR
4	I	2	LEU
4	I	5	VAL
4	I	25	ARG
4	I	29	ARG

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Mol	Chain	Res	Type
4	I	39	GLN
4	J	2	LEU
4	J	4	LYS
4	J	5	VAL
4	J	17	ILE
4	J	24	GLU
4	J	42	ARG
4	J	50	MET
4	J	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	64	GLN
1	A	77	GLN
1	A	197	GLN
1	A	322	ASN
1	A	359	ASN
1	A	436	HIS
1	A	438	GLN
1	A	449	GLN
1	A	466	GLN
1	A	480	HIS
1	A	517	ASN
2	B	1019	ASN
2	B	1040	HIS
2	B	1050	GLN
2	B	1073	GLN
2	B	1087	GLN
2	B	1101	ASN
2	B	1202	ASN
2	B	1219	ASN
2	B	1254	GLN
2	B	1324	ASN
2	B	1326	GLN
2	B	1356	GLN
2	B	1368	ASN
2	B	2032	HIS
2	B	2119	ASN
2	B	2139	HIS
2	B	2210	GLN

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Mol	Chain	Res	Type
2	B	2227	HIS
2	B	2270	GLN
2	B	2272	ASN
2	B	2282	GLN
2	B	2296	ASN
2	B	2348	GLN
2	B	2354	GLN
2	B	2362	GLN
2	B	2375	GLN
2	B	2432	GLN
3	C	10	GLN
3	C	35	GLN
3	C	39	ASN
3	C	59	ASN
3	C	84	GLN
3	C	146	ASN
4	I	49	GLN
4	J	41	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
7	ATP	B	103	5	32,33,33	1.42	5 (15%)	48,52,52	2.02	11 (22%)

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
7	ATP	B	103	5	-	6/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	103	ATP	PA-O3A	-2.80	1.56	1.59
7	B	103	ATP	C2-N1	2.72	1.38	1.33
7	B	103	ATP	O2'-C2'	-2.39	1.37	1.43
7	B	103	ATP	C4-N3	2.32	1.38	1.34
7	B	103	ATP	C2-N3	2.23	1.37	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	103	ATP	N3-C2-N1	-5.95	119.57	128.58
7	B	103	ATP	C5-N7-C8	4.87	111.10	103.45
7	B	103	ATP	C4-C5-N7	-4.47	105.47	110.58
7	B	103	ATP	N9-C8-N7	-4.42	107.67	113.94
7	B	103	ATP	C2-N3-C4	3.31	119.92	111.83
7	B	103	ATP	C6-C5-N7	3.12	138.11	132.09
7	B	103	ATP	C5-C4-N3	-3.11	122.43	126.72
7	B	103	ATP	O2B-PB-O3A	2.58	114.25	107.27
7	B	103	ATP	C4-N9-C8	2.53	108.39	105.74
7	B	103	ATP	O2B-PB-O3B	2.46	113.92	107.27
7	B	103	ATP	O2'-C2'-C3'	2.37	119.41	111.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

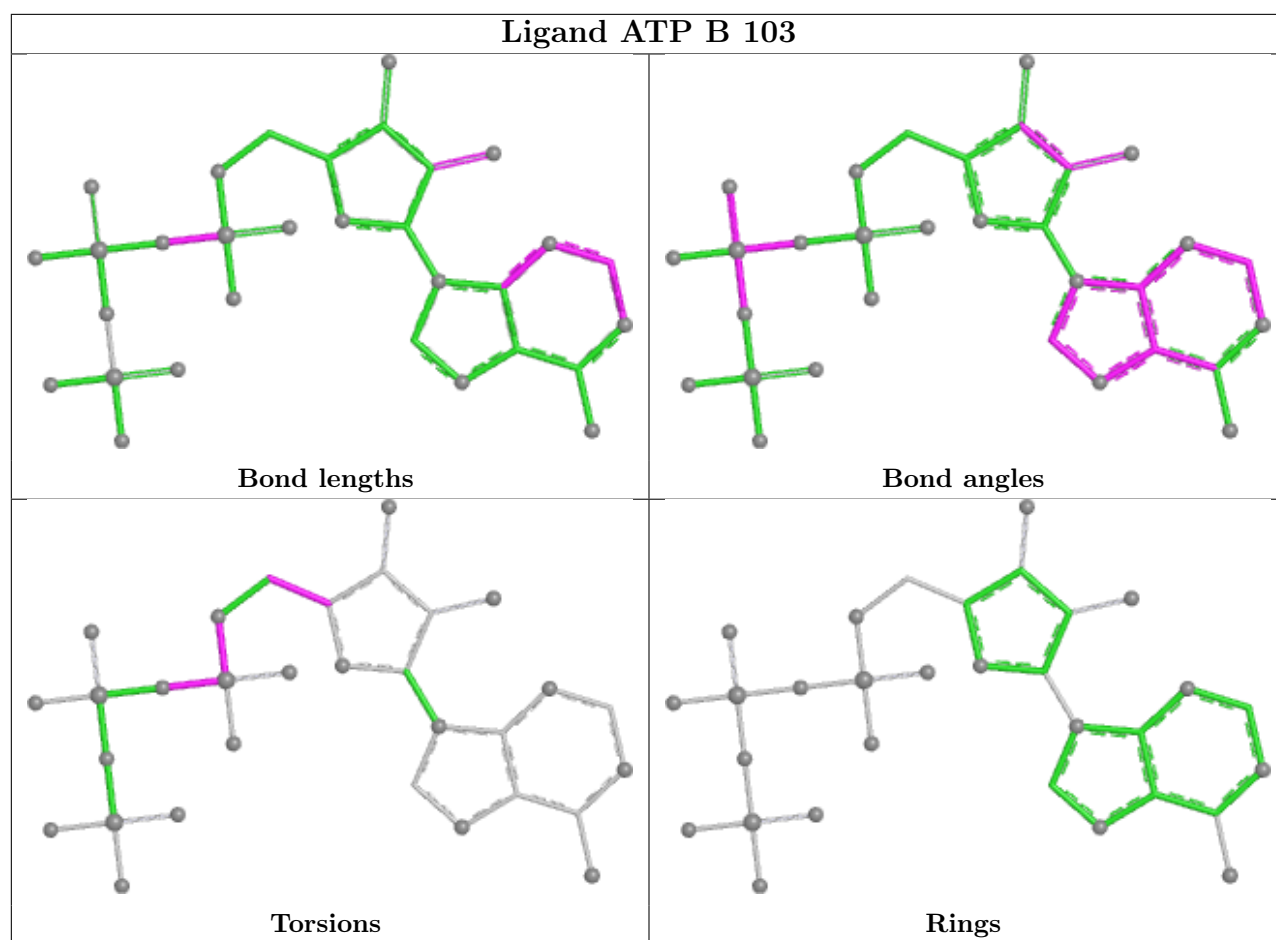
Mol	Chain	Res	Type	Atoms
7	B	103	ATP	C5'-O5'-PA-O1A
7	B	103	ATP	C5'-O5'-PA-O2A
7	B	103	ATP	C5'-O5'-PA-O3A
7	B	103	ATP	PB-O3A-PA-O1A
7	B	103	ATP	PB-O3A-PA-O2A
7	B	103	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	103	ATP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	530/536 (98%)	0.15	9 (1%) 69 60	42, 72, 111, 142	0
2	B	789/805 (98%)	0.53	91 (11%) 9 7	37, 77, 145, 150	0
3	C	176/180 (97%)	0.10	0 100 100	48, 75, 96, 104	2 (1%)
4	I	76/81 (93%)	0.12	0 100 100	43, 73, 92, 100	0
4	J	76/81 (93%)	2.85	49 (64%) 0 0	95, 142, 149, 150	0
All	All	1647/1683 (97%)	0.45	149 (9%) 15 11	37, 76, 142, 150	2 (0%)

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	J	67	LEU	9.4
1	A	7	LEU	8.5
4	J	5	VAL	7.1
4	J	26	ILE	7.0
4	J	13	ILE	6.8
4	J	43	LEU	6.3
4	J	66	VAL	6.0
4	J	30	VAL	5.9
4	J	3	ILE	5.2
4	J	50	MET	5.2
2	B	1097	ALA	5.1
4	J	37	PRO	4.8
2	B	1094	THR	4.7
2	B	1062	PHE	4.7
2	B	1111	VAL	4.5
2	B	1113	ALA	4.4
2	B	1276	LEU	4.3
2	B	1294	VAL	4.3
2	B	1277	ALA	4.2
2	B	1054	THR	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	1221	GLY	4.1
2	B	1247	VAL	4.1
4	J	36	ILE	4.0
2	B	1008	LEU	4.0
4	J	70	VAL	4.0
2	B	1321	THR	3.9
2	B	1034	ILE	3.9
2	B	1022	ALA	3.9
4	J	56	ALA	3.9
2	B	1291	LEU	3.8
4	J	69	LEU	3.8
2	B	1095	TRP	3.8
4	J	62	LEU	3.8
2	B	1304	ALA	3.8
4	J	59	TYR	3.7
2	B	1109	ILE	3.6
4	J	15	ILE	3.6
4	J	27	LYS	3.6
4	J	8	LEU	3.6
4	J	38	PRO	3.5
4	J	20	THR	3.5
2	B	1150	PHE	3.5
2	B	1009	VAL	3.5
4	J	2	LEU	3.5
4	J	48	LYS	3.5
2	B	1224	ALA	3.5
4	J	17	ILE	3.4
4	J	44	ILE	3.4
2	B	1245	VAL	3.4
1	A	8	LEU	3.3
2	B	1320	ALA	3.3
2	B	1006	GLY	3.3
4	J	7	THR	3.3
4	J	19	PRO	3.2
2	B	1061	ILE	3.2
4	J	4	LYS	3.2
4	J	61	ILE	3.2
2	B	1024	VAL	3.2
1	A	448	TYR	3.1
2	B	1021	LEU	3.1
2	B	1110	ALA	3.1
2	B	1223	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	1127	PRO	3.1
4	J	1	MET	3.0
4	J	40	GLN	2.9
2	B	1259	PHE	2.9
4	J	76	GLY	2.9
4	J	23	VAL	2.9
2	B	1133	ILE	2.9
2	B	1105	ILE	2.9
2	B	1055	GLY	2.9
2	B	1227	ILE	2.9
2	B	1147	ALA	2.8
2	B	1093	PHE	2.8
2	B	1226	THR	2.8
2	B	1219	ASN	2.8
2	B	1108	PRO	2.8
4	J	57	ALA	2.7
2	B	1263	LEU	2.7
2	B	1123	LEU	2.7
2	B	1119	ASN	2.7
4	J	21	ASP	2.7
4	J	73	LEU	2.7
4	J	41	GLN	2.7
2	B	1281	LEU	2.7
2	B	1265	ALA	2.7
2	B	1177	TYR	2.7
2	B	1115	SER	2.7
2	B	1060	ILE	2.6
2	B	1122	LEU	2.6
4	J	22	LYS	2.5
4	J	55	THR	2.5
2	B	1179	ILE	2.5
2	B	1262	VAL	2.5
4	J	9	THR	2.5
4	J	65	SER	2.5
2	B	1112	GLU	2.5
2	B	1270	ALA	2.5
1	A	201	LEU	2.4
2	B	1267	ILE	2.4
2	B	1035	LYS	2.4
4	J	33	LYS	2.4
2	B	1149	MET	2.4
2	B	1130	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
4	J	45	TYR	2.4
2	B	1017	GLY	2.4
2	B	1218	PHE	2.4
2	B	1011	TRP	2.4
2	B	1158	THR	2.4
4	J	47	GLY	2.4
2	B	1205	MET	2.4
2	B	1199	LEU	2.4
2	B	1255	PRO	2.4
2	B	1142	ALA	2.3
1	A	297	ILE	2.3
2	B	1120	LYS	2.3
1	A	264	ASN	2.3
2	B	1117	ILE	2.3
4	J	10	GLY	2.3
2	B	1012	ILE	2.2
2	B	2211	VAL	2.2
2	B	1251	PHE	2.2
2	B	1295	ASN	2.2
2	B	1156	TYR	2.2
2	B	1256	SER	2.2
2	B	1230	PRO	2.2
2	B	1032	THR	2.2
2	B	1063	TRP	2.2
2	B	1233	TRP	2.2
2	B	1298	LYS	2.2
2	B	1216	ALA	2.2
2	B	1134	PRO	2.2
2	B	1157	PHE	2.2
2	B	1036	VAL	2.1
4	J	52	ASP	2.1
1	A	80	SER	2.1
4	J	63	GLY	2.1
4	J	54	LYS	2.1
2	B	1096	ASP	2.1
2	B	1280	PHE	2.1
2	B	1347	ALA	2.1
2	B	1091	TYR	2.1
4	J	60	LYS	2.0
1	A	353	ASP	2.0
1	A	249	GLN	2.0
2	B	1028	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	1225	MET	2.0
2	B	1100	TYR	2.0
2	B	1241	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

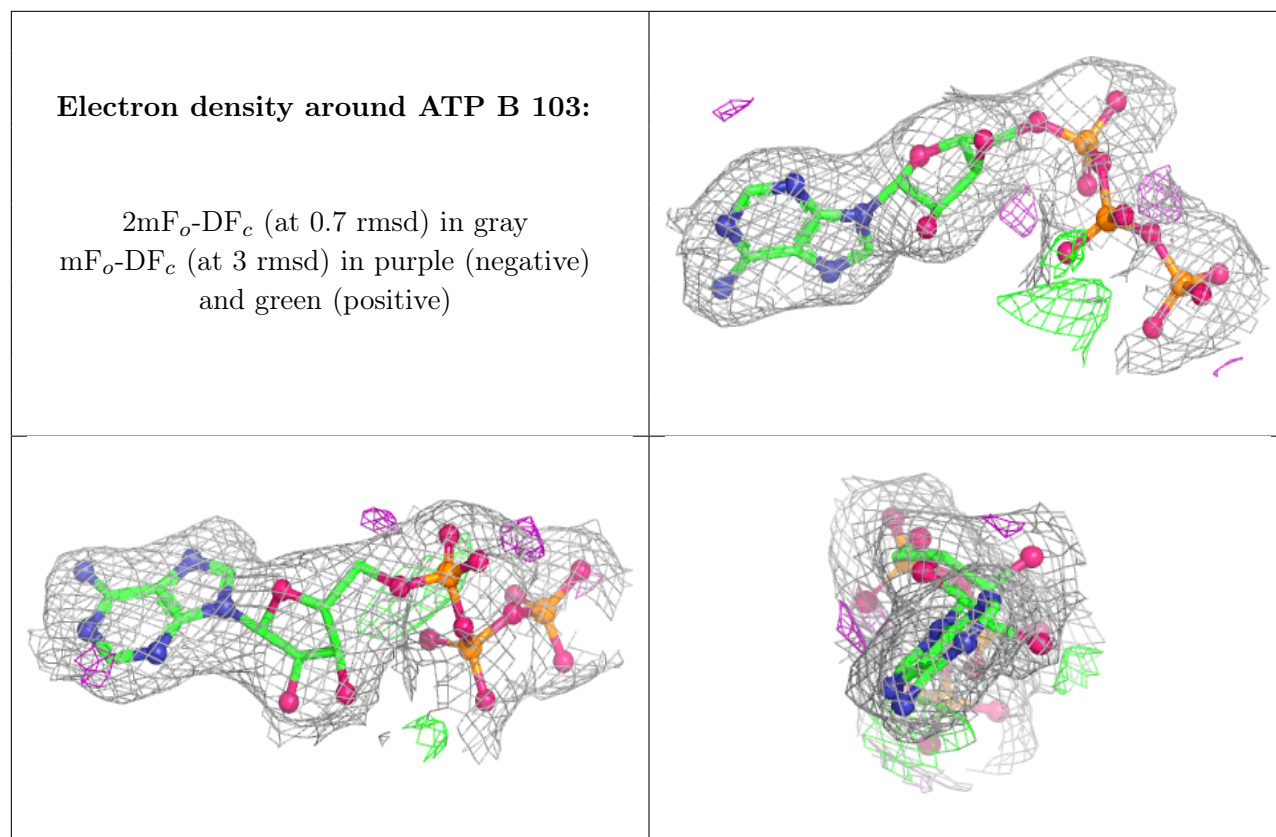
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	B	101	1/1	0.78	0.26	68,68,68,68	0
7	ATP	B	103	31/31	0.95	0.08	60,62,70,73	0
6	ZN	B	102	1/1	0.99	0.20	61,61,61,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.