



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:04 PM UTC

PDB ID : 2G5I / pdb_00002g5i
Title : Structure of tRNA-Dependent Amidotransferase GatCAB complexed with ADP-AlF₄
Authors : Nakamura, A.; Yao, M.; Tanaka, I.
Deposited on : 2006-02-23
Resolution : 3.35 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

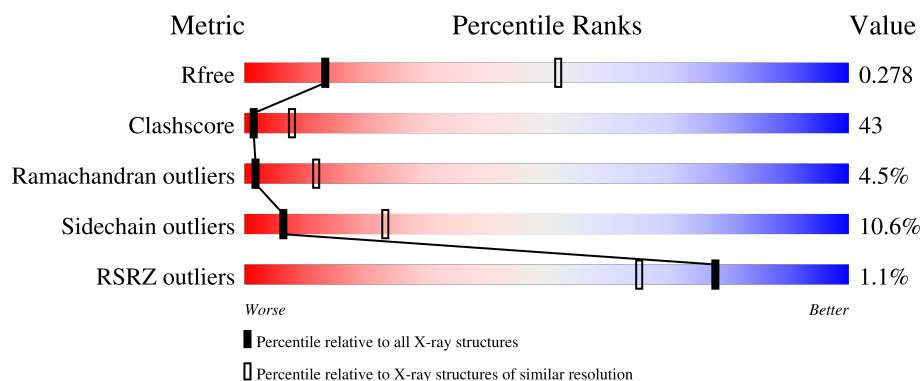
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	485	
2	B	483	
3	C	100	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7874 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 Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3716	2359	605	739	13			

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	410	Total	C	N	O	S	0	0	0
			3266	2058	550	645	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	476	LEU	-	expression tag	UNP P64201
B	477	GLU	-	expression tag	UNP P64201
B	478	HIS	-	expression tag	UNP P64201
B	479	HIS	-	expression tag	UNP P64201
B	480	HIS	-	expression tag	UNP P64201
B	481	HIS	-	expression tag	UNP P64201
B	482	HIS	-	expression tag	UNP P64201
B	483	HIS	-	expression tag	UNP P64201

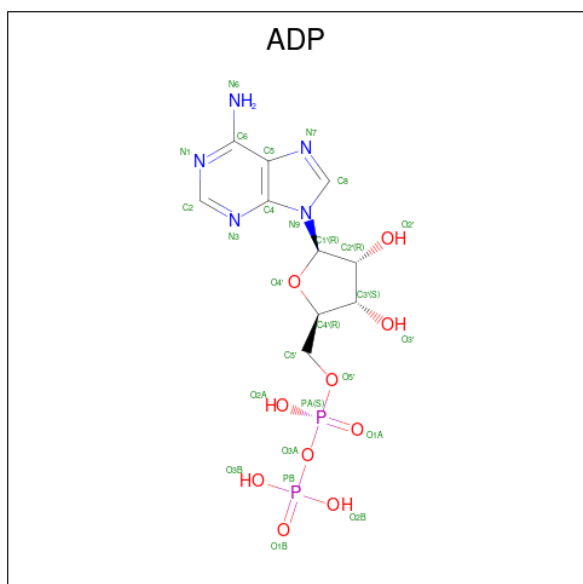
- Molecule 3 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	98	Total	C	N	O	S	0	0	0
			774	476	129	167	2			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

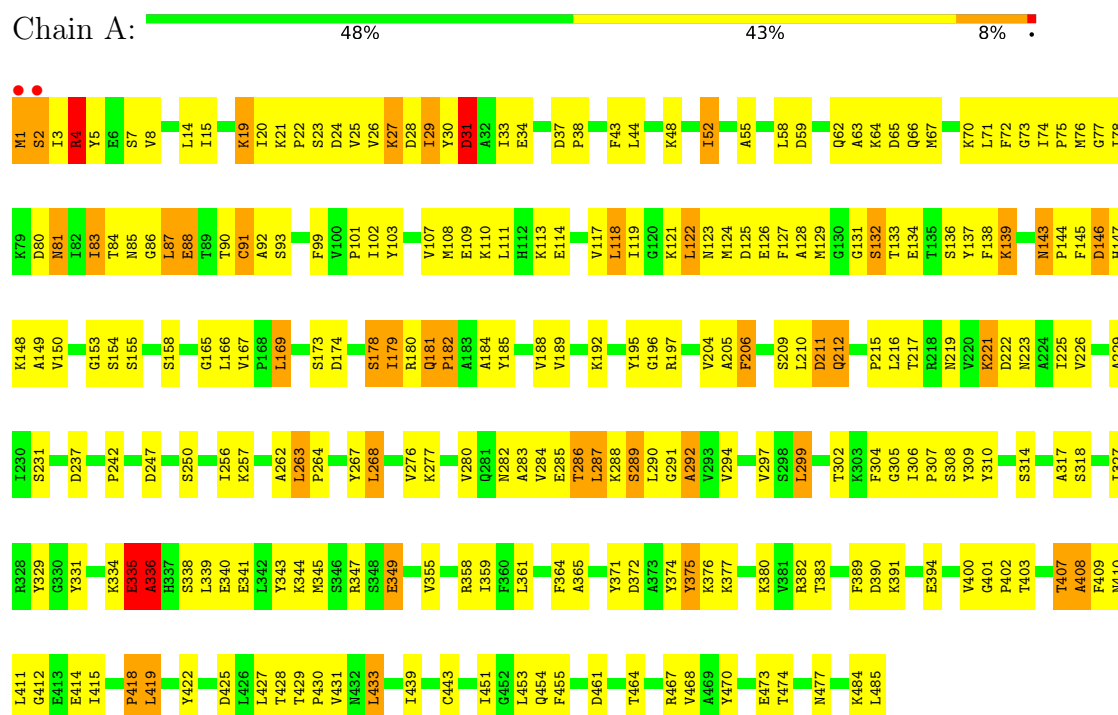
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	42	Total	O	0	0
			42	42		
6	B	39	Total	O	0	0
			39	39		
6	C	9	Total	O	0	0
			9	9		

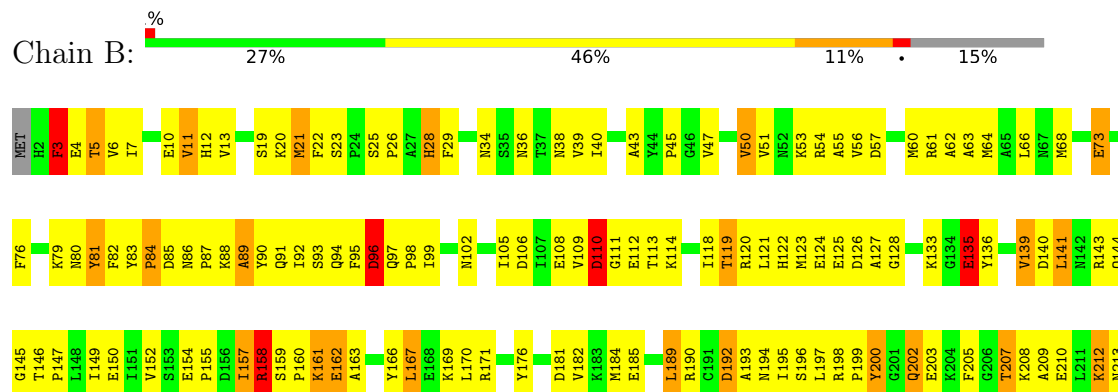
3 Residue-property plots

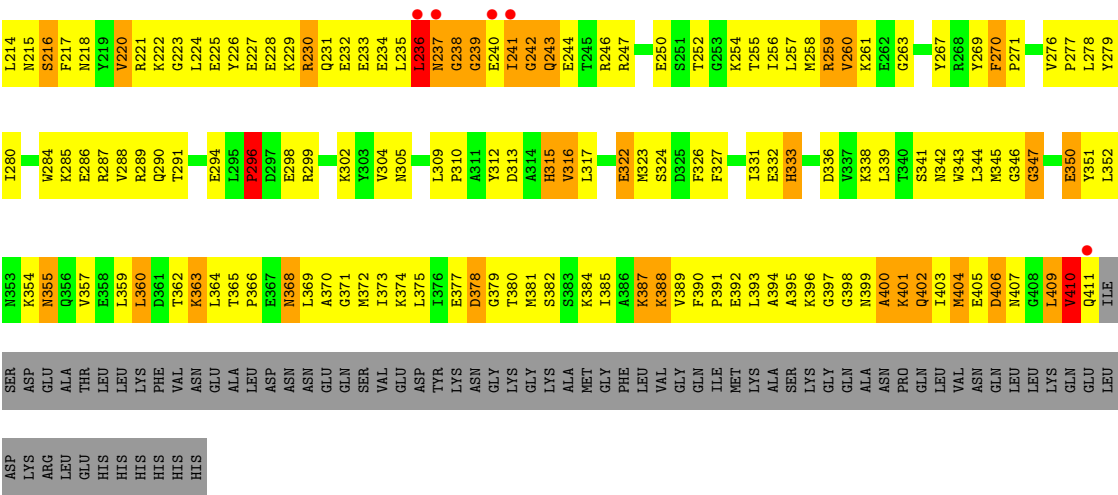
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutamyl-tRNA(Gln) amidotransferase subunit A



• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B





● Molecule 3: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.86Å 85.28Å 183.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.35 20.00 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-3.35) 97.8 (20.00-3.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.297 0.217 , 0.278	Depositor DCC
R_{free} test set	2800 reflections (14.41%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 12.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7874	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: MG, ADP

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	0.41	1/3784 (0.0%)	1.04	19/5116 (0.4%)
2	B	0.42	0/3329	1.11	27/4495 (0.6%)
3	C	0.63	1/782 (0.1%)	1.25	10/1056 (0.9%)
All	All	0.44	2/7895 (0.0%)	1.09	56/10667 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	100	ALA	C-OXT	5.42	1.34	1.23
1	A	286	THR	CA-CB	5.12	1.62	1.53

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	GLN	N-CA-C	-14.12	88.53	110.42
3	C	99	ASP	N-CA-C	-11.21	93.99	111.02
3	C	98	GLU	N-CA-C	10.74	124.96	112.93
3	C	16	ALA	N-CA-C	-9.43	98.08	110.53
3	C	100	ALA	CA-C-O	9.32	148.96	121.00
2	B	158	ARG	N-CA-C	8.03	122.86	112.26
2	B	406	ASP	N-CA-C	-7.82	103.63	113.02
2	B	236	LEU	N-CA-C	-7.58	104.16	113.41
2	B	238	GLY	N-CA-C	-7.50	95.40	113.18
1	A	299	LEU	CA-C-N	7.44	127.80	119.32
1	A	299	LEU	C-N-CA	7.44	127.80	119.32
1	A	336	ALA	N-CA-C	7.13	125.98	110.80
2	B	86	ASN	CA-C-N	6.88	128.44	119.84
2	B	86	ASN	C-N-CA	6.88	128.44	119.84
2	B	21	MET	N-CA-C	6.59	118.46	111.28
1	A	88	GLU	N-CA-C	-6.42	97.13	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	SER	N-CA-C	-6.39	104.36	111.71
2	B	378	ASP	N-CA-C	-6.39	105.62	113.41
2	B	203	GLU	N-CA-C	-6.34	103.44	112.13
3	C	98	GLU	CA-CB-CG	-6.30	101.49	114.10
2	B	379	GLY	N-CA-C	-6.24	107.27	114.69
2	B	96	ASP	N-CA-C	6.19	119.30	111.69
1	A	179	ILE	CB-CA-C	-6.09	104.94	110.91
1	A	292	ALA	N-CA-C	6.02	118.72	110.24
1	A	335	GLU	CA-C-N	6.01	133.02	121.54
1	A	335	GLU	C-N-CA	6.01	133.02	121.54
1	A	205	ALA	N-CA-C	5.97	118.00	110.24
2	B	3	PHE	N-CA-C	5.97	118.00	110.24
1	A	81	ASN	N-CA-C	-5.92	104.71	112.41
2	B	112	GLU	N-CA-C	5.87	118.79	109.81
3	C	60	GLN	N-CA-C	5.82	117.24	108.46
1	A	336	ALA	CA-C-N	-5.75	111.48	122.53
1	A	336	ALA	C-N-CA	-5.75	111.48	122.53
2	B	51	VAL	N-CA-C	5.75	117.14	109.37
2	B	139	VAL	N-CA-C	5.60	116.37	108.36
1	A	19	LYS	N-CA-C	-5.58	106.61	113.41
2	B	133	LYS	N-CA-C	5.57	117.75	107.73
1	A	286	THR	N-CA-C	-5.51	105.17	112.34
3	C	37	ASP	N-CA-C	-5.49	105.30	111.28
2	B	332	GLU	N-CA-C	-5.43	106.69	113.15
2	B	400	ALA	N-CA-C	5.40	116.97	111.14
1	A	91	CYS	N-CA-C	-5.38	105.80	112.47
2	B	89	ALA	N-CA-C	-5.36	106.11	113.56
2	B	239	GLY	N-CA-C	5.32	125.78	113.18
2	B	29	PHE	N-CA-C	5.30	118.20	109.72
2	B	135	GLU	N-CA-C	-5.29	105.16	111.03
2	B	162	GLU	N-CA-C	-5.29	105.59	111.36
3	C	100	ALA	N-CA-C	-5.27	96.24	111.00
2	B	102	ASN	N-CA-C	5.25	118.56	111.17
3	C	97	GLU	CA-C-N	-5.24	113.95	122.65
3	C	97	GLU	C-N-CA	-5.24	113.95	122.65
2	B	192	ASP	N-CA-C	-5.14	100.79	109.07
1	A	109	GLU	N-CA-C	-5.09	105.62	111.07
1	A	31	ASP	N-CA-C	-5.09	105.62	111.07
1	A	407	THR	N-CA-C	-5.03	102.62	110.42
2	B	11	VAL	N-CA-C	5.02	114.80	107.37

There are no chirality outliers.

There are no planarity outliers.

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	3716	0	3709	260	0
2	B	3266	0	3214	359	0
3	C	774	0	753	81	0
4	B	1	0	0	0	0
5	B	27	0	12	2	0
6	A	42	0	0	3	0
6	B	39	0	0	13	0
6	C	9	0	0	4	0
All	All	7874	0	7688	668	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 43.

All (668) 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:A:341:GLU:HG3	3:C:97:GLU:OE2	1.41	1.19
1:A:83:ILE:HD12	1:A:103:TYR:CE1	1.82	1.13
2:B:259:ARG:HG2	2:B:259:ARG:HH11	1.13	1.07
2:B:407:ASN:OD1	6:B:605:HOH:O	1.76	1.02
2:B:60:MET:HE2	2:B:288:VAL:HG21	1.39	1.01
1:A:1:MET:HA	1:A:4:ARG:HB3	1.40	1.01
2:B:192:ASP:HB3	6:B:624:HOH:O	1.60	1.00
3:C:22:PRO:O	3:C:24:GLU:N	1.96	0.97
2:B:401:LYS:H	2:B:401:LYS:HD2	1.30	0.97
2:B:259:ARG:NH1	6:B:635:HOH:O	1.98	0.96
1:A:150:VAL:HG12	1:A:411:LEU:HD23	1.48	0.95
2:B:259:ARG:HH11	2:B:259:ARG:CG	1.77	0.93
1:A:93:SER:HB2	1:A:126:GLU:HG3	1.48	0.92
2:B:213:ASN:ND2	2:B:215:ASN:HD21	1.66	0.92
3:C:22:PRO:O	3:C:25:THR:N	2.02	0.92
2:B:26:PRO:HB2	2:B:36:ASN:HD21	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ASP:OD2	1:A:250:SER:HB3	1.68	0.91
1:A:361:LEU:HG	3:C:35:ILE:HG21	1.49	0.91
2:B:210:GLU:OE2	2:B:212:LYS:CE	2.19	0.90
2:B:231:GLN:CB	2:B:241:ILE:HD12	2.02	0.90
2:B:231:GLN:HB2	2:B:241:ILE:HD12	1.53	0.89
2:B:3:PHE:HE1	2:B:232:GLU:HG3	1.38	0.87
1:A:27:LYS:HE2	1:A:27:LYS:HA	1.55	0.87
3:C:98:GLU:OE2	3:C:98:GLU:HA	1.58	0.87
2:B:368:ASN:ND2	2:B:393:LEU:HD21	1.90	0.87
2:B:259:ARG:NH2	6:B:635:HOH:O	2.07	0.86
2:B:109:VAL:HG11	2:B:162:GLU:HG2	1.57	0.86
2:B:372:MET:HE2	2:B:389:VAL:HG23	1.55	0.85
2:B:215:ASN:ND2	2:B:250:GLU:OE2	2.09	0.85
1:A:123:ASN:ND2	1:A:124:MET:H	1.74	0.85
5:B:601:ADP:H5'2	5:B:601:ADP:O1B	1.77	0.85
3:C:99:ASP:C	3:C:100:ALA:OXT	2.05	0.85
3:C:95:MET:HB2	3:C:100:ALA:HB2	1.58	0.85
1:A:429:THR:OG1	1:A:430:PRO:HD3	1.77	0.84
2:B:326:PHE:CD2	2:B:359:LEU:HD11	2.13	0.84
2:B:34:ASN:HD21	2:B:140:ASP:HA	1.44	0.83
1:A:338:SER:OG	3:C:97:GLU:OE2	1.96	0.83
2:B:98:PRO:HG3	2:B:120:ARG:NH2	1.94	0.82
2:B:259:ARG:CZ	6:B:635:HOH:O	2.26	0.82
2:B:351:TYR:OH	2:B:395:ALA:HB3	1.79	0.82
3:C:93:THR:C	3:C:95:MET:H	1.87	0.82
1:A:484:LYS:O	1:A:485:LEU:HB2	1.78	0.82
2:B:34:ASN:ND2	2:B:140:ASP:HA	1.95	0.81
2:B:213:ASN:HD21	2:B:215:ASN:HD21	1.28	0.80
1:A:29:ILE:HG21	1:A:119:ILE:HG12	1.62	0.80
3:C:20:ILE:O	3:C:20:ILE:HD12	1.80	0.80
1:A:129:MET:SD	1:A:358:ARG:HG3	2.21	0.80
1:A:280:VAL:HG21	1:A:402:PRO:HB3	1.61	0.80
3:C:95:MET:HB2	3:C:100:ALA:CB	2.11	0.80
2:B:143:ARG:O	2:B:146:THR:HG23	1.83	0.79
2:B:3:PHE:HB3	2:B:199:PRO:HA	1.64	0.79
3:C:93:THR:O	3:C:95:MET:N	2.17	0.78
2:B:365:THR:HG23	2:B:368:ASN:H	1.47	0.78
2:B:3:PHE:HD2	2:B:199:PRO:HG3	1.47	0.78
2:B:336:ASP:HB3	2:B:339:LEU:HB2	1.65	0.77
2:B:56:VAL:HG22	2:B:123:MET:HE1	1.65	0.77
2:B:259:ARG:HG2	2:B:259:ARG:NH1	1.96	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:LYS:H	2:B:395:ALA:HA	1.50	0.76
2:B:140:ASP:HB2	3:C:88:GLN:HE21	1.50	0.76
2:B:364:LEU:HB2	2:B:368:ASN:HD21	1.50	0.76
1:A:1:MET:SD	1:A:1:MET:N	2.59	0.75
2:B:257:LEU:HD21	2:B:259:ARG:O	1.85	0.75
2:B:7:ILE:HG22	2:B:195:ILE:HA	1.68	0.75
1:A:81:ASN:HB3	1:A:124:MET:SD	2.27	0.75
1:A:1:MET:O	1:A:4:ARG:N	2.19	0.75
1:A:143:ASN:ND2	1:A:145:PHE:H	1.85	0.75
1:A:153:GLY:H	1:A:181:GLN:HE22	1.34	0.75
2:B:227:GLU:HB2	2:B:255:THR:HG21	1.69	0.74
2:B:96:ASP:O	2:B:98:PRO:HD2	1.87	0.74
2:B:154:GLU:HG3	2:B:155:PRO:HD2	1.68	0.74
2:B:390:PHE:HB3	2:B:391:PRO:HD3	1.69	0.74
2:B:410:VAL:O	2:B:411:GLN:HB2	1.87	0.74
2:B:5:THR:HG21	2:B:228:GLU:OE2	1.88	0.73
2:B:233:GLU:HG3	2:B:234:GLU:N	2.04	0.73
1:A:195:TYR:HA	1:A:212:GLN:OE1	1.88	0.73
2:B:210:GLU:OE2	2:B:212:LYS:HE2	1.87	0.73
1:A:153:GLY:H	1:A:181:GLN:NE2	1.85	0.73
1:A:402:PRO:HG2	1:A:427:LEU:HD13	1.70	0.72
1:A:169:LEU:HD12	1:A:169:LEU:C	2.14	0.72
1:A:62:GLN:HG3	1:A:67:MET:HE3	1.70	0.72
1:A:84:THR:CG2	1:A:121:LYS:HE3	2.18	0.72
2:B:21:MET:HE3	2:B:21:MET:O	1.90	0.71
2:B:98:PRO:HG3	2:B:120:ARG:CZ	2.20	0.71
2:B:384:LYS:HE2	2:B:384:LYS:HA	1.70	0.71
1:A:374:TYR:CE2	3:C:36:LEU:HD22	2.26	0.71
2:B:236:LEU:O	2:B:236:LEU:CD1	2.38	0.71
2:B:256:ILE:HD12	6:B:630:HOH:O	1.90	0.71
2:B:207:THR:OG1	2:B:242:GLY:HA2	1.90	0.71
2:B:60:MET:HE2	2:B:288:VAL:CG2	2.19	0.71
3:C:35:ILE:O	3:C:38:PHE:HB3	1.91	0.71
3:C:96:ASN:O	3:C:100:ALA:HB3	1.90	0.71
1:A:169:LEU:HD12	1:A:169:LEU:O	1.91	0.70
1:A:341:GLU:CG	3:C:97:GLU:OE2	2.32	0.70
1:A:22:PRO:HD2	1:A:59:ASP:OD1	1.92	0.70
2:B:355:ASN:O	2:B:357:VAL:HG23	1.92	0.70
2:B:388:LYS:HA	2:B:388:LYS:HZ3	1.57	0.70
2:B:246:ARG:HD3	2:B:255:THR:HB	1.73	0.69
2:B:85:ASP:O	2:B:127:ALA:HB1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:ARG:NH1	2:B:259:ARG:CG	2.43	0.69
2:B:258:MET:O	2:B:259:ARG:CD	2.40	0.69
1:A:1:MET:CA	1:A:4:ARG:HB3	2.20	0.69
2:B:83:TYR:CD2	2:B:84:PRO:HD2	2.28	0.69
1:A:143:ASN:C	1:A:143:ASN:HD22	2.01	0.69
2:B:388:LYS:HA	2:B:388:LYS:NZ	2.08	0.69
2:B:13:VAL:HB	2:B:149:ILE:HG13	1.73	0.69
1:A:334:LYS:C	1:A:336:ALA:H	1.99	0.69
2:B:374:LYS:HA	2:B:377:GLU:HG2	1.74	0.69
2:B:365:THR:HG22	2:B:368:ASN:OD1	1.94	0.68
2:B:13:VAL:HB	2:B:149:ILE:CG1	2.24	0.68
2:B:360:LEU:N	2:B:360:LEU:HD12	2.09	0.68
1:A:127:PHE:O	6:A:502:HOH:O	2.10	0.68
1:A:341:GLU:HG3	3:C:97:GLU:CD	2.19	0.67
2:B:217:PHE:O	2:B:220:VAL:HG22	1.94	0.67
3:C:93:THR:C	3:C:95:MET:N	2.51	0.67
2:B:20:LYS:HB3	2:B:145:GLY:O	1.94	0.67
1:A:276:VAL:HA	1:A:451:ILE:HD13	1.76	0.67
2:B:3:PHE:CD1	2:B:3:PHE:N	2.62	0.67
1:A:14:LEU:HD12	1:A:19:LYS:HD2	1.76	0.67
1:A:188:VAL:HG13	1:A:217:THR:O	1.95	0.67
1:A:419:LEU:HD23	6:A:491:HOH:O	1.94	0.66
1:A:26:VAL:HG21	1:A:55:ALA:HB2	1.76	0.66
1:A:263:LEU:HD23	1:A:400:VAL:HG13	1.77	0.66
2:B:231:GLN:O	2:B:235:LEU:HD13	1.95	0.66
2:B:374:LYS:HA	2:B:377:GLU:OE2	1.95	0.66
2:B:139:VAL:HB	3:C:89:PHE:HB2	1.76	0.66
1:A:143:ASN:HD22	1:A:145:PHE:H	1.42	0.66
2:B:372:MET:CG	2:B:381:MET:HE1	2.25	0.66
2:B:258:MET:O	2:B:259:ARG:HD2	1.95	0.66
1:A:280:VAL:O	1:A:284:VAL:HG23	1.96	0.66
2:B:22:PHE:O	2:B:50:VAL:HG23	1.94	0.66
1:A:340:GLU:HB3	3:C:97:GLU:OE1	1.96	0.66
2:B:210:GLU:OE2	2:B:212:LYS:HE3	1.93	0.65
1:A:310:TYR:HE2	1:A:422:TYR:CZ	2.15	0.65
2:B:6:VAL:HG13	2:B:158:ARG:HH22	1.62	0.65
1:A:215:PRO:C	1:A:216:LEU:HD12	2.21	0.65
2:B:231:GLN:HB3	2:B:241:ILE:HD12	1.79	0.65
2:B:233:GLU:HG3	2:B:234:GLU:H	1.60	0.65
2:B:136:TYR:CD1	3:C:90:LYS:HE3	2.32	0.65
2:B:393:LEU:HD23	2:B:393:LEU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ARG:HE	2:B:182:VAL:HG23	1.62	0.65
3:C:33:GLU:OE2	6:C:103:HOH:O	2.14	0.65
2:B:242:GLY:O	2:B:244:GLU:N	2.28	0.64
2:B:372:MET:HG2	2:B:381:MET:HE1	1.77	0.64
1:A:131:GLY:HA2	1:A:153:GLY:HA3	1.80	0.64
1:A:284:VAL:O	1:A:287:LEU:HB2	1.97	0.64
2:B:271:PRO:HG3	3:C:54:TYR:CE1	2.32	0.64
3:C:97:GLU:O	3:C:98:GLU:CD	2.40	0.64
2:B:236:LEU:O	2:B:236:LEU:HD13	1.98	0.64
2:B:362:THR:OG1	2:B:364:LEU:HD23	1.98	0.64
2:B:280:ILE:HA	2:B:284:TRP:CE3	2.33	0.64
2:B:309:LEU:HG	2:B:310:PRO:HD2	1.78	0.64
2:B:246:ARG:HD3	2:B:255:THR:CB	2.28	0.64
1:A:284:VAL:HG13	1:A:294:VAL:HG11	1.80	0.64
1:A:345:MET:O	1:A:349:GLU:HB2	1.97	0.64
2:B:184:MET:HE2	2:B:216:SER:N	2.13	0.63
2:B:352:LEU:HD21	2:B:359:LEU:HB2	1.80	0.63
2:B:80:ASN:O	2:B:81:TYR:HB3	1.98	0.63
2:B:294:GLU:OE2	2:B:302:LYS:HE2	1.98	0.63
1:A:143:ASN:HD22	1:A:144:PRO:N	1.96	0.63
1:A:83:ILE:CD1	1:A:103:TYR:CE1	2.72	0.63
2:B:105:ILE:HD11	2:B:166:TYR:CD1	2.34	0.63
2:B:279:TYR:H	3:C:61:ASN:HD21	1.46	0.63
2:B:198:ARG:HG3	2:B:202:GLN:HB3	1.80	0.62
1:A:226:VAL:O	1:A:229:ALA:HB3	1.99	0.62
2:B:3:PHE:HA	6:B:638:HOH:O	1.99	0.62
1:A:197:ARG:HD2	1:A:231:SER:HB3	1.82	0.62
2:B:363:LYS:HG2	2:B:397:GLY:O	2.00	0.62
1:A:83:ILE:HD12	1:A:103:TYR:HE1	1.56	0.62
2:B:109:VAL:CG1	2:B:162:GLU:HG2	2.29	0.62
2:B:218:ASN:O	2:B:221:ARG:HB2	1.99	0.62
3:C:96:ASN:O	3:C:100:ALA:OXT	2.18	0.62
1:A:23:SER:HA	1:A:55:ALA:HB1	1.81	0.62
2:B:64:MET:HE1	2:B:288:VAL:HG23	1.81	0.61
1:A:174:ASP:HB3	1:A:192:LYS:HG3	1.82	0.61
2:B:11:VAL:HA	2:B:190:ARG:O	2.00	0.61
2:B:53:LYS:HB2	3:C:63:LEU:HB3	1.82	0.61
1:A:84:THR:OG1	1:A:121:LYS:HE3	2.00	0.61
1:A:306:ILE:N	1:A:307:PRO:HD2	2.16	0.61
2:B:171:ARG:NE	2:B:182:VAL:HG23	2.15	0.61
1:A:87:LEU:HD12	1:A:118:LEU:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:THR:O	2:B:7:ILE:HG23	2.00	0.61
2:B:216:SER:O	2:B:220:VAL:HG13	2.01	0.61
2:B:3:PHE:CE1	2:B:232:GLU:HG3	2.29	0.61
1:A:169:LEU:C	1:A:169:LEU:CD1	2.74	0.60
2:B:62:ALA:O	2:B:66:LEU:HD13	2.01	0.60
2:B:109:VAL:O	2:B:110:ASP:C	2.44	0.60
2:B:312:TYR:O	2:B:315:HIS:HB3	2.02	0.60
1:A:1:MET:O	1:A:2:SER:C	2.45	0.60
2:B:68:MET:HE1	2:B:120:ARG:C	2.25	0.60
2:B:79:LYS:HG3	2:B:269:TYR:CE1	2.37	0.60
2:B:236:LEU:O	2:B:236:LEU:HD12	2.02	0.60
2:B:365:THR:N	2:B:368:ASN:OD1	2.33	0.60
2:B:121:LEU:HA	2:B:150:GLU:O	2.02	0.59
1:A:58:LEU:HD23	1:A:73:GLY:HA2	1.84	0.59
1:A:470:TYR:O	1:A:474:THR:HG23	2.02	0.59
2:B:368:ASN:HD22	2:B:368:ASN:C	2.10	0.59
2:B:382:SER:OG	2:B:385:ILE:HD13	2.02	0.59
2:B:323:MET:HE2	2:B:344:LEU:HD22	1.83	0.59
3:C:22:PRO:O	3:C:23:GLU:C	2.45	0.59
1:A:146:ASP:OD1	1:A:148:LYS:HB2	2.03	0.59
1:A:149:ALA:HA	1:A:410:ASN:HA	1.85	0.59
2:B:66:LEU:HD23	2:B:118:ILE:HD13	1.84	0.59
2:B:240:GLU:O	2:B:241:ILE:HG12	2.02	0.59
1:A:21:LYS:HB2	1:A:24:ASP:OD2	2.03	0.59
1:A:125:ASP:CG	1:A:133:THR:HA	2.28	0.59
1:A:179:ILE:C	1:A:182:PRO:HD2	2.28	0.58
2:B:229:LYS:O	2:B:230:ARG:C	2.46	0.58
3:C:3:LYS:HE3	3:C:4:VAL:H	1.68	0.58
2:B:309:LEU:HG	2:B:310:PRO:CD	2.32	0.58
2:B:198:ARG:CG	2:B:202:GLN:HB3	2.34	0.58
2:B:393:LEU:HD23	2:B:393:LEU:C	2.28	0.58
2:B:171:ARG:HG2	2:B:182:VAL:HB	1.85	0.58
2:B:399:ASN:OD1	2:B:401:LYS:HD2	2.04	0.58
2:B:372:MET:HE1	2:B:390:PHE:HB2	1.86	0.58
1:A:14:LEU:O	1:A:20:ILE:HG22	2.04	0.57
1:A:257:LYS:HA	1:A:291:GLY:HA3	1.85	0.57
2:B:387:LYS:HZ2	2:B:387:LYS:HB2	1.69	0.57
1:A:99:PHE:CE1	1:A:101:PRO:HG3	2.39	0.57
1:A:15:ILE:O	1:A:67:MET:HE1	2.04	0.57
1:A:126:GLU:O	1:A:127:PHE:HB2	2.02	0.57
1:A:210:LEU:HD13	1:A:382:ARG:NH2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:VAL:HG11	2:B:205:PHE:CE1	2.40	0.57
2:B:121:LEU:HD23	2:B:121:LEU:O	2.05	0.57
2:B:338:LYS:HE3	2:B:342:ASN:HD21	1.67	0.57
1:A:402:PRO:HG2	1:A:427:LEU:CD1	2.34	0.56
2:B:199:PRO:HD2	2:B:202:GLN:NE2	2.19	0.56
1:A:14:LEU:CD1	1:A:19:LYS:HD2	2.36	0.56
1:A:44:LEU:HD23	1:A:139:LYS:HD3	1.87	0.56
1:A:263:LEU:HD23	1:A:400:VAL:CG1	2.35	0.56
2:B:171:ARG:NE	2:B:182:VAL:CG2	2.68	0.56
1:A:123:ASN:ND2	1:A:124:MET:N	2.50	0.56
1:A:174:ASP:HA	1:A:178:SER:HB2	1.88	0.56
2:B:10:GLU:HB3	2:B:192:ASP:HB2	1.87	0.56
2:B:323:MET:O	2:B:324:SER:C	2.48	0.56
1:A:285:GLU:C	1:A:287:LEU:N	2.61	0.56
2:B:91:GLN:OE1	2:B:124:GLU:HB3	2.05	0.56
1:A:174:ASP:HB2	1:A:179:ILE:HG13	1.87	0.56
1:A:181:GLN:HE21	1:A:181:GLN:C	2.13	0.56
1:A:331:TYR:CE2	1:A:349:GLU:HB3	2.40	0.56
2:B:236:LEU:CD1	2:B:236:LEU:C	2.79	0.56
2:B:199:PRO:HA	6:B:638:HOH:O	2.05	0.56
3:C:8:GLU:OE1	3:C:8:GLU:HA	2.05	0.56
2:B:215:ASN:O	2:B:216:SER:HB2	2.06	0.56
1:A:403:THR:OG1	1:A:454:GLN:HB2	2.06	0.55
2:B:258:MET:O	2:B:259:ARG:HD3	2.06	0.55
1:A:257:LYS:HB3	1:A:291:GLY:HA3	1.87	0.55
2:B:34:ASN:OD1	3:C:89:PHE:HE2	1.88	0.55
2:B:368:ASN:ND2	2:B:368:ASN:C	2.65	0.55
1:A:364:PHE:HD2	3:C:12:ILE:HD11	1.71	0.55
2:B:167:LEU:HD23	2:B:217:PHE:HD1	1.71	0.55
2:B:243:GLN:HG3	2:B:261:LYS:HG3	1.88	0.55
1:A:1:MET:O	1:A:4:ARG:CB	2.54	0.55
1:A:188:VAL:HG12	1:A:189:VAL:N	2.22	0.55
1:A:347:ARG:HD3	3:C:17:ARG:O	2.06	0.55
2:B:34:ASN:ND2	2:B:141:LEU:H	2.04	0.55
1:A:123:ASN:HD22	1:A:124:MET:H	1.54	0.55
2:B:88:LYS:O	2:B:89:ALA:HB3	2.06	0.55
2:B:149:ILE:HG13	2:B:149:ILE:O	2.05	0.55
2:B:387:LYS:HB2	2:B:387:LYS:NZ	2.22	0.55
1:A:166:LEU:O	1:A:167:VAL:HG13	2.07	0.55
1:A:76:MET:CB	1:A:169:LEU:HD11	2.37	0.55
1:A:304:PHE:O	1:A:307:PRO:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:HB	2:B:194:ASN:O	2.06	0.54
1:A:58:LEU:CD2	1:A:73:GLY:HA2	2.38	0.54
1:A:181:GLN:NE2	1:A:181:GLN:C	2.65	0.54
1:A:256:ILE:HG21	1:A:468:VAL:HA	1.88	0.54
1:A:307:PRO:HG2	1:A:308:SER:H	1.72	0.54
1:A:102:ILE:CG2	3:C:76:LEU:HD22	2.37	0.54
1:A:90:THR:C	1:A:92:ALA:N	2.64	0.54
2:B:341:SER:OG	2:B:345:MET:HE2	2.07	0.54
2:B:5:THR:HG21	2:B:228:GLU:HG3	1.89	0.54
2:B:85:ASP:HB2	2:B:128:GLY:C	2.33	0.54
2:B:401:LYS:H	2:B:401:LYS:CD	2.10	0.54
1:A:153:GLY:N	1:A:181:GLN:HE22	2.03	0.54
1:A:412:GLY:HA2	1:A:415:ILE:CG2	2.38	0.54
2:B:7:ILE:CG2	2:B:195:ILE:HG13	2.38	0.54
2:B:63:ALA:HB2	2:B:121:LEU:HD22	1.90	0.54
1:A:33:ILE:HD11	1:A:119:ILE:HG21	1.89	0.54
1:A:62:GLN:HG3	1:A:67:MET:CE	2.38	0.54
2:B:184:MET:HE2	2:B:215:ASN:C	2.33	0.54
2:B:247:ARG:HB3	2:B:258:MET:HE2	1.90	0.54
2:B:374:LYS:O	2:B:377:GLU:HG2	2.08	0.54
1:A:76:MET:HG2	1:A:117:VAL:O	2.08	0.53
2:B:284:TRP:O	2:B:288:VAL:HG22	2.08	0.53
2:B:210:GLU:CG	6:B:624:HOH:O	2.56	0.53
2:B:360:LEU:HD12	2:B:360:LEU:H	1.73	0.53
1:A:339:LEU:HD11	1:A:343:TYR:HE2	1.73	0.53
2:B:34:ASN:HD21	2:B:141:LEU:H	1.57	0.53
2:B:209:ALA:HA	2:B:244:GLU:O	2.09	0.53
2:B:213:ASN:ND2	2:B:215:ASN:ND2	2.48	0.53
2:B:280:ILE:HA	2:B:284:TRP:HE3	1.74	0.53
1:A:355:VAL:O	1:A:359:ILE:HG13	2.09	0.53
2:B:241:ILE:HA	2:B:244:GLU:OE1	2.09	0.53
1:A:146:ASP:C	1:A:148:LYS:H	2.16	0.53
1:A:1:MET:CE	1:A:31:ASP:HB3	2.38	0.53
1:A:180:ARG:NH1	1:A:431:VAL:HG21	2.24	0.53
1:A:419:LEU:HA	1:A:422:TYR:HD2	1.74	0.53
2:B:25:SER:OG	2:B:38:ASN:ND2	2.42	0.53
2:B:66:LEU:HD23	2:B:118:ILE:CD1	2.39	0.53
2:B:354:LYS:O	2:B:355:ASN:ND2	2.42	0.53
1:A:257:LYS:HA	1:A:291:GLY:C	2.34	0.52
2:B:200:TYR:N	6:B:638:HOH:O	2.36	0.52
2:B:246:ARG:NH1	2:B:255:THR:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:ASP:CG	6:C:106:HOH:O	2.51	0.52
1:A:37:ASP:OD2	1:A:43:PHE:HB2	2.08	0.52
1:A:4:ARG:HD2	1:A:5:TYR:CE2	2.44	0.52
2:B:157:ILE:HD13	2:B:163:ALA:N	2.25	0.52
2:B:169:LYS:O	2:B:170:LEU:C	2.53	0.52
2:B:196:SER:HB2	2:B:207:THR:C	2.34	0.52
2:B:359:LEU:O	2:B:359:LEU:HD22	2.10	0.52
1:A:380:LYS:O	1:A:383:THR:HB	2.10	0.52
2:B:79:LYS:HE2	2:B:269:TYR:OH	2.09	0.52
2:B:160:PRO:HG2	2:B:161:LYS:HD3	1.92	0.52
1:A:125:ASP:OD1	1:A:133:THR:HA	2.10	0.52
1:A:429:THR:O	1:A:433:LEU:HD22	2.10	0.52
2:B:195:ILE:O	2:B:208:LYS:HA	2.09	0.52
1:A:382:ARG:HG3	1:A:433:LEU:HB3	1.91	0.52
1:A:1:MET:HA	1:A:4:ARG:CB	2.28	0.52
1:A:1:MET:O	1:A:4:ARG:HB3	2.10	0.52
1:A:216:LEU:HD12	1:A:216:LEU:N	2.24	0.52
2:B:26:PRO:HD3	3:C:69:ILE:O	2.10	0.52
2:B:82:PHE:CD1	3:C:17:ARG:HG2	2.45	0.52
2:B:43:ALA:CB	2:B:87:PRO:HB2	2.40	0.52
2:B:66:LEU:HD12	2:B:66:LEU:N	2.25	0.52
1:A:264:PRO:HG2	1:A:267:TYR:CG	2.45	0.51
2:B:80:ASN:HB2	2:B:267:TYR:O	2.10	0.51
2:B:106:ASP:O	2:B:169:LYS:NZ	2.43	0.51
2:B:184:MET:CE	2:B:216:SER:N	2.72	0.51
2:B:304:VAL:HG12	2:B:305:ASN:OD1	2.09	0.51
2:B:336:ASP:OD2	2:B:339:LEU:HD23	2.10	0.51
2:B:385:ILE:N	2:B:385:ILE:HD12	2.25	0.51
2:B:405:GLU:C	2:B:407:ASN:H	2.19	0.51
1:A:179:ILE:HG23	1:A:216:LEU:HD11	1.91	0.51
3:C:97:GLU:O	3:C:98:GLU:OE2	2.29	0.51
2:B:82:PHE:CE1	3:C:17:ARG:HG2	2.45	0.51
2:B:193:ALA:CB	2:B:224:LEU:HD11	2.40	0.51
2:B:184:MET:HG2	2:B:189:LEU:O	2.11	0.51
2:B:212:LYS:HD3	2:B:212:LYS:N	2.26	0.51
2:B:286:GLU:O	2:B:289:ARG:N	2.42	0.51
2:B:363:LYS:HB2	2:B:396:LYS:H	1.76	0.51
2:B:181:ASP:C	2:B:182:VAL:HG22	2.36	0.51
3:C:97:GLU:O	3:C:100:ALA:OXT	2.28	0.51
1:A:108:MET:HE1	1:A:111:LEU:HD12	1.93	0.51
2:B:286:GLU:O	2:B:287:ARG:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ILE:HD13	3:C:91:VAL:HG11	1.93	0.51
1:A:364:PHE:CD1	1:A:364:PHE:C	2.89	0.51
2:B:252:THR:OG1	2:B:254:LYS:HG3	2.11	0.51
3:C:34:SER:O	3:C:35:ILE:C	2.52	0.51
1:A:443:CYS:HB3	1:A:453:LEU:HB2	1.93	0.51
2:B:256:ILE:CD1	6:B:630:HOH:O	2.54	0.51
1:A:391:LYS:O	1:A:394:GLU:HB2	2.11	0.50
2:B:140:ASP:HB2	3:C:88:GLN:NE2	2.23	0.50
2:B:285:LYS:O	2:B:289:ARG:HB2	2.10	0.50
3:C:22:PRO:C	3:C:24:GLU:N	2.68	0.50
1:A:3:ILE:HD12	1:A:3:ILE:C	2.36	0.50
2:B:365:THR:CG2	2:B:368:ASN:H	2.18	0.50
2:B:371:GLY:O	2:B:375:LEU:HG	2.11	0.50
3:C:97:GLU:O	3:C:98:GLU:OE1	2.30	0.50
1:A:188:VAL:CG1	1:A:189:VAL:N	2.75	0.50
1:A:219:ASN:HD21	1:A:222:ASP:CG	2.19	0.50
1:A:4:ARG:HD3	1:A:165:GLY:O	2.11	0.50
1:A:110:LYS:O	1:A:113:LYS:HB3	2.10	0.50
2:B:157:ILE:HD12	2:B:159:SER:H	1.76	0.50
2:B:96:ASP:O	2:B:98:PRO:CD	2.58	0.50
1:A:1:MET:HE1	1:A:31:ASP:OD2	2.12	0.50
1:A:84:THR:HG21	1:A:121:LYS:HE3	1.93	0.49
2:B:299:ARG:O	2:B:302:LYS:HB2	2.13	0.49
1:A:37:ASP:N	1:A:38:PRO:CD	2.75	0.49
1:A:83:ILE:HD12	1:A:103:TYR:CZ	2.42	0.49
1:A:102:ILE:HG21	3:C:76:LEU:HD22	1.93	0.49
2:B:28:HIS:ND1	2:B:28:HIS:N	2.61	0.49
2:B:109:VAL:HG11	2:B:162:GLU:CG	2.38	0.49
2:B:154:GLU:CG	2:B:155:PRO:HD2	2.41	0.49
2:B:197:LEU:HD22	2:B:231:GLN:HG3	1.93	0.49
2:B:227:GLU:HA	2:B:230:ARG:HB2	1.93	0.49
2:B:286:GLU:O	2:B:289:ARG:HB3	2.12	0.49
2:B:381:MET:HG3	2:B:385:ILE:HB	1.93	0.49
1:A:62:GLN:HE21	1:A:67:MET:HE1	1.78	0.49
1:A:338:SER:OG	3:C:97:GLU:CD	2.55	0.49
2:B:171:ARG:HD3	2:B:171:ARG:C	2.37	0.49
1:A:256:ILE:HD12	1:A:292:ALA:HB2	1.94	0.49
1:A:285:GLU:C	1:A:287:LEU:H	2.21	0.49
2:B:374:LYS:HA	2:B:377:GLU:CG	2.42	0.49
1:A:146:ASP:O	1:A:148:LYS:N	2.46	0.49
2:B:109:VAL:O	2:B:111:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:GLU:O	2:B:241:ILE:CG1	2.61	0.49
2:B:315:HIS:O	2:B:316:VAL:C	2.56	0.49
1:A:464:THR:O	1:A:467:ARG:HB3	2.13	0.49
2:B:229:LYS:O	2:B:232:GLU:N	2.46	0.49
2:B:399:ASN:HB3	2:B:402:GLN:CG	2.42	0.49
3:C:3:LYS:CE	3:C:4:VAL:H	2.25	0.49
1:A:77:GLY:C	1:A:122:LEU:HD22	2.38	0.48
1:A:103:TYR:HB3	2:B:39:VAL:HG11	1.94	0.48
1:A:2:SER:HB2	1:A:28:ASP:OD2	2.14	0.48
1:A:174:ASP:HB2	1:A:179:ILE:CG1	2.42	0.48
2:B:43:ALA:HB2	2:B:87:PRO:HB2	1.95	0.48
2:B:3:PHE:HB3	2:B:199:PRO:CA	2.40	0.48
2:B:214:LEU:HD22	2:B:220:VAL:HA	1.93	0.48
1:A:85:ASN:HD22	1:A:86:GLY:H	1.61	0.48
1:A:85:ASN:HD22	1:A:86:GLY:N	2.10	0.48
1:A:288:LYS:O	1:A:290:LEU:O	2.32	0.48
1:A:375:TYR:O	1:A:376:LYS:C	2.55	0.48
1:A:473:GLU:O	1:A:477:ASN:ND2	2.39	0.48
2:B:385:ILE:HG12	2:B:409:LEU:HD12	1.95	0.48
1:A:317:ALA:O	1:A:318:SER:C	2.55	0.48
1:A:419:LEU:HA	1:A:422:TYR:CD2	2.48	0.48
2:B:241:ILE:O	2:B:242:GLY:O	2.32	0.48
1:A:185:TYR:CE2	1:A:408:ALA:HA	2.48	0.48
2:B:38:ASN:OD1	2:B:38:ASN:C	2.56	0.48
1:A:150:VAL:HG22	1:A:409:PHE:O	2.14	0.48
1:A:283:ALA:O	1:A:284:VAL:C	2.57	0.48
3:C:99:ASP:HB2	6:C:106:HOH:O	2.12	0.48
2:B:12:HIS:NE2	2:B:150:GLU:HG3	2.28	0.48
3:C:7:GLU:CD	3:C:7:GLU:H	2.21	0.48
3:C:36:LEU:O	3:C:40:LYS:HG2	2.14	0.48
1:A:48:LYS:O	1:A:52:ILE:HD12	2.13	0.48
1:A:185:TYR:CD2	1:A:408:ALA:HA	2.48	0.48
1:A:264:PRO:HG3	1:A:267:TYR:CD2	2.48	0.48
1:A:257:LYS:CA	1:A:291:GLY:HA3	2.44	0.48
2:B:96:ASP:C	2:B:98:PRO:CD	2.87	0.48
2:B:105:ILE:HD11	2:B:166:TYR:CE1	2.49	0.48
3:C:99:ASP:CB	6:C:106:HOH:O	2.62	0.48
1:A:285:GLU:O	1:A:288:LYS:N	2.47	0.47
1:A:76:MET:HB2	1:A:169:LEU:HD11	1.95	0.47
3:C:3:LYS:HE3	3:C:4:VAL:N	2.28	0.47
3:C:33:GLU:OE1	3:C:33:GLU:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:TYR:CZ	1:A:48:LYS:HA	2.49	0.47
2:B:40:ILE:HA	2:B:47:VAL:HG21	1.95	0.47
2:B:20:LYS:HA	2:B:147:PRO:HD3	1.96	0.47
2:B:93:SER:OG	2:B:94:GLN:N	2.47	0.47
3:C:20:ILE:HD13	3:C:25:THR:OG1	2.14	0.47
3:C:99:ASP:O	3:C:100:ALA:C	2.56	0.47
1:A:37:ASP:N	1:A:38:PRO:HD3	2.29	0.47
1:A:72:PHE:C	1:A:72:PHE:CD1	2.93	0.47
1:A:181:GLN:HB3	1:A:182:PRO:HD3	1.97	0.47
1:A:264:PRO:CG	1:A:267:TYR:CD2	2.97	0.47
2:B:7:ILE:HG22	2:B:195:ILE:HG13	1.97	0.47
2:B:139:VAL:HG12	2:B:141:LEU:HD13	1.97	0.47
3:C:10:GLU:O	3:C:14:ASN:HB2	2.15	0.47
1:A:30:TYR:O	1:A:34:GLU:HG3	2.15	0.47
1:A:221:LYS:O	1:A:225:ILE:HG13	2.14	0.47
1:A:372:ASP:HA	1:A:376:LYS:HB3	1.96	0.47
2:B:372:MET:HE1	2:B:390:PHE:CA	2.45	0.47
2:B:399:ASN:HB3	2:B:402:GLN:HG3	1.96	0.47
1:A:71:LEU:O	1:A:74:ILE:HG12	2.15	0.47
1:A:91:CYS:SG	1:A:204:VAL:HG21	2.55	0.47
2:B:90:TYR:O	2:B:90:TYR:CD2	2.67	0.47
1:A:365:ALA:O	1:A:371:TYR:HA	2.15	0.46
2:B:199:PRO:O	2:B:200:TYR:C	2.59	0.46
2:B:210:GLU:CD	2:B:212:LYS:HE3	2.39	0.46
3:C:76:LEU:O	3:C:77:ALA:C	2.58	0.46
2:B:176:TYR:CZ	2:B:296:PRO:HG3	2.50	0.46
2:B:225:GLU:O	2:B:228:GLU:HB3	2.15	0.46
1:A:155:SER:O	1:A:158:SER:HB2	2.16	0.46
1:A:376:LYS:O	1:A:377:LYS:C	2.58	0.46
2:B:171:ARG:HE	2:B:182:VAL:CG2	2.28	0.46
1:A:181:GLN:HE21	1:A:182:PRO:N	2.12	0.46
2:B:171:ARG:HD2	6:B:606:HOH:O	2.15	0.46
2:B:193:ALA:HB1	2:B:224:LEU:HD11	1.97	0.46
2:B:246:ARG:HD3	2:B:255:THR:OG1	2.15	0.46
2:B:294:GLU:O	2:B:299:ARG:HD2	2.16	0.46
1:A:361:LEU:HD22	1:A:361:LEU:O	2.15	0.46
2:B:94:GLN:HB2	2:B:122:HIS:HB2	1.97	0.46
2:B:95:PHE:CD1	2:B:96:ASP:OD1	2.69	0.46
3:C:59:LEU:O	3:C:60:GLN:HG3	2.15	0.46
1:A:407:THR:O	1:A:408:ALA:C	2.57	0.46
2:B:73:GLU:C	2:B:97:GLN:NE2	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:GLU:C	2:B:135:GLU:CD	2.84	0.46
2:B:372:MET:HE1	2:B:390:PHE:CB	2.44	0.46
1:A:412:GLY:HA2	1:A:415:ILE:HG22	1.98	0.46
2:B:7:ILE:O	2:B:157:ILE:HG13	2.16	0.46
2:B:369:LEU:O	2:B:370:ALA:C	2.59	0.46
3:C:38:PHE:CD1	3:C:41:GLN:NE2	2.84	0.46
1:A:15:ILE:HG12	1:A:20:ILE:HG23	1.98	0.46
1:A:154:SER:OG	1:A:178:SER:HB3	2.15	0.46
2:B:403:ILE:O	2:B:407:ASN:HB3	2.15	0.46
1:A:77:GLY:C	1:A:78:ILE:HD12	2.41	0.46
2:B:387:LYS:NZ	2:B:387:LYS:CB	2.79	0.46
2:B:399:ASN:OD1	2:B:400:ALA:N	2.48	0.46
1:A:62:GLN:CG	1:A:67:MET:HE3	2.42	0.45
1:A:285:GLU:O	1:A:287:LEU:N	2.48	0.45
2:B:96:ASP:C	2:B:98:PRO:HD3	2.41	0.45
2:B:122:HIS:O	2:B:149:ILE:HA	2.16	0.45
2:B:126:ASP:HB3	2:B:146:THR:OG1	2.16	0.45
1:A:23:SER:HA	1:A:55:ALA:CB	2.46	0.45
1:A:329:TYR:CZ	2:B:45:PRO:HD3	2.51	0.45
2:B:331:ILE:C	2:B:333:HIS:H	2.23	0.45
2:B:368:ASN:HD22	2:B:393:LEU:HD21	1.78	0.45
1:A:150:VAL:CG1	1:A:411:LEU:HD23	2.32	0.45
1:A:206:PHE:CD1	1:A:206:PHE:C	2.94	0.45
2:B:227:GLU:O	2:B:231:GLN:HG2	2.17	0.45
1:A:283:ALA:O	1:A:287:LEU:N	2.50	0.45
1:A:400:VAL:HG22	1:A:401:GLY:N	2.32	0.45
2:B:410:VAL:O	2:B:411:GLN:CB	2.62	0.45
1:A:7:SER:HB2	1:A:222:ASP:OD2	2.17	0.45
2:B:276:VAL:HG21	3:C:59:LEU:HB3	1.98	0.45
3:C:15:LEU:HD23	3:C:15:LEU:HA	1.77	0.45
1:A:242:PRO:HD3	3:C:59:LEU:HD21	1.98	0.45
2:B:197:LEU:N	2:B:197:LEU:CD1	2.80	0.45
2:B:236:LEU:HD12	2:B:236:LEU:C	2.42	0.45
1:A:8:VAL:N	1:A:222:ASP:OD2	2.49	0.45
2:B:91:GLN:HG3	2:B:125:GLU:HG3	1.98	0.44
2:B:121:LEU:HD23	2:B:121:LEU:C	2.41	0.44
2:B:241:ILE:CG1	2:B:241:ILE:O	2.65	0.44
2:B:257:LEU:C	2:B:257:LEU:HD13	2.42	0.44
1:A:173:SER:C	1:A:179:ILE:HG13	2.42	0.44
2:B:278:LEU:HA	3:C:61:ASN:ND2	2.33	0.44
3:C:32:LEU:HD13	3:C:32:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:ILE:HD12	3:C:76:LEU:CB	2.46	0.44
1:A:439:ILE:HG22	1:A:455:PHE:HB2	1.99	0.44
2:B:22:PHE:O	2:B:50:VAL:CG2	2.64	0.44
2:B:240:GLU:C	2:B:242:GLY:N	2.71	0.44
2:B:322:GLU:H	2:B:322:GLU:CD	2.24	0.44
2:B:343:TRP:CD1	2:B:373:ILE:HD12	2.52	0.44
2:B:381:MET:SD	2:B:389:VAL:HG21	2.57	0.44
1:A:146:ASP:C	1:A:148:LYS:N	2.74	0.44
1:A:262:ALA:HB1	1:A:297:VAL:CG2	2.47	0.44
1:A:90:THR:C	1:A:92:ALA:H	2.25	0.44
1:A:419:LEU:H	1:A:419:LEU:HD22	1.82	0.44
2:B:22:PHE:CE2	2:B:92:ILE:HB	2.53	0.44
2:B:365:THR:H	2:B:368:ASN:CG	2.26	0.44
2:B:402:GLN:NE2	2:B:406:ASP:OD1	2.50	0.44
1:A:309:TYR:CD2	1:A:310:TYR:N	2.86	0.44
2:B:365:THR:O	2:B:366:PRO:C	2.60	0.44
1:A:1:MET:C	1:A:4:ARG:HB3	2.43	0.44
1:A:29:ILE:HG21	1:A:119:ILE:CG1	2.43	0.44
2:B:34:ASN:OD1	3:C:89:PHE:CE2	2.68	0.44
2:B:241:ILE:HG12	2:B:241:ILE:O	2.14	0.44
2:B:365:THR:OG1	2:B:366:PRO:HD2	2.18	0.44
2:B:372:MET:HE1	2:B:390:PHE:HA	1.97	0.44
1:A:63:ALA:C	1:A:65:ASP:H	2.26	0.44
1:A:282:ASN:O	1:A:285:GLU:N	2.51	0.44
2:B:385:ILE:HG21	2:B:404:MET:CE	2.48	0.44
1:A:70:LYS:HD2	6:A:511:HOH:O	2.17	0.43
2:B:54:ARG:O	2:B:55:ALA:C	2.61	0.43
2:B:61:ARG:HD3	2:B:291:THR:OG1	2.17	0.43
2:B:160:PRO:HB3	2:B:224:LEU:HB3	1.99	0.43
2:B:347:GLY:O	2:B:350:GLU:HB2	2.18	0.43
2:B:192:ASP:OD2	2:B:212:LYS:HE2	2.18	0.43
2:B:239:GLY:HA2	6:B:620:HOH:O	2.18	0.43
1:A:78:ILE:HG12	1:A:108:MET:CE	2.48	0.43
2:B:54:ARG:O	2:B:57:ASP:HB2	2.17	0.43
2:B:167:LEU:HG	2:B:217:PHE:CE1	2.53	0.43
1:A:111:LEU:O	1:A:114:GLU:N	2.51	0.43
1:A:380:LYS:O	1:A:383:THR:N	2.51	0.43
1:A:418:PRO:HG2	1:A:419:LEU:HD22	2.00	0.43
2:B:68:MET:SD	2:B:121:LEU:HB3	2.59	0.43
2:B:119:THR:HG23	2:B:152:VAL:O	2.19	0.43
2:B:323:MET:O	2:B:326:PHE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ILE:HD13	1:A:101:PRO:HB3	2.00	0.43
1:A:126:GLU:HG2	1:A:355:VAL:HG21	2.01	0.43
2:B:76:PHE:CD1	2:B:76:PHE:N	2.87	0.43
3:C:70:LYS:HG3	3:C:71:GLY:N	2.32	0.43
1:A:22:PRO:O	1:A:26:VAL:HG23	2.18	0.43
1:A:59:ASP:O	1:A:62:GLN:HB3	2.19	0.43
2:B:233:GLU:O	2:B:236:LEU:HB3	2.18	0.43
1:A:7:SER:O	1:A:8:VAL:C	2.62	0.43
1:A:136:SER:C	1:A:138:PHE:H	2.27	0.43
1:A:257:LYS:HA	1:A:291:GLY:CA	2.48	0.43
2:B:323:MET:HE2	2:B:344:LEU:HB3	2.00	0.43
2:B:363:LYS:CB	2:B:396:LYS:H	2.32	0.43
1:A:23:SER:CA	1:A:55:ALA:HB1	2.48	0.43
1:A:75:PRO:HB3	1:A:119:ILE:CD1	2.48	0.43
1:A:180:ARG:NH2	1:A:428:THR:HB	2.34	0.43
1:A:107:VAL:HG23	1:A:108:MET:N	2.32	0.43
1:A:306:ILE:HA	1:A:429:THR:HG21	2.01	0.43
1:A:335:GLU:CD	1:A:335:GLU:H	2.26	0.43
2:B:56:VAL:O	2:B:60:MET:HG2	2.19	0.43
2:B:231:GLN:HB2	2:B:241:ILE:CD1	2.38	0.43
2:B:313:ASP:OD2	2:B:345:MET:HE1	2.19	0.43
2:B:402:GLN:O	2:B:406:ASP:N	2.47	0.43
3:C:72:ILE:HD12	3:C:76:LEU:HB3	2.01	0.43
2:B:237:ASN:C	2:B:238:GLY:O	2.60	0.42
2:B:220:VAL:O	2:B:224:LEU:HB2	2.18	0.42
2:B:280:ILE:O	2:B:285:LYS:HE3	2.18	0.42
2:B:64:MET:CE	2:B:288:VAL:HG23	2.48	0.42
3:C:17:ARG:O	3:C:18:LEU:HD23	2.19	0.42
1:A:210:LEU:CD1	1:A:382:ARG:NH2	2.82	0.42
1:A:314:SER:HB3	1:A:358:ARG:O	2.20	0.42
2:B:181:ASP:C	2:B:182:VAL:CG2	2.92	0.42
2:B:359:LEU:HD13	2:B:359:LEU:C	2.44	0.42
1:A:285:GLU:O	1:A:286:THR:C	2.62	0.42
2:B:21:MET:HB2	2:B:147:PRO:HA	2.01	0.42
2:B:378:ASP:HB3	2:B:380:THR:OG1	2.19	0.42
3:C:5:THR:O	3:C:6:ARG:C	2.63	0.42
1:A:209:SER:OG	1:A:210:LEU:HD22	2.19	0.42
1:A:237:ASP:OD1	1:A:237:ASP:C	2.61	0.42
2:B:181:ASP:O	2:B:182:VAL:CG2	2.67	0.42
2:B:226:TYR:CZ	2:B:254:LYS:HB3	2.55	0.42
1:A:284:VAL:O	1:A:287:LEU:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:PHE:HD2	2:B:359:LEU:HD11	1.77	0.42
2:B:360:LEU:N	2:B:360:LEU:CD1	2.81	0.42
1:A:389:PHE:O	1:A:390:ASP:C	2.62	0.42
2:B:7:ILE:CG2	2:B:195:ILE:HA	2.45	0.42
2:B:60:MET:O	2:B:64:MET:HG3	2.20	0.42
2:B:73:GLU:O	2:B:97:GLN:NE2	2.49	0.42
3:C:9:VAL:CG1	3:C:25:THR:HG23	2.49	0.42
1:A:44:LEU:CD2	1:A:139:LYS:HD3	2.49	0.42
2:B:160:PRO:HG3	2:B:225:GLU:HB3	2.02	0.42
2:B:184:MET:CG	2:B:189:LEU:HD12	2.50	0.42
1:A:276:VAL:O	1:A:277:LYS:C	2.63	0.41
1:A:282:ASN:O	1:A:283:ALA:C	2.62	0.41
2:B:6:VAL:O	5:B:601:ADP:H2	2.02	0.41
2:B:401:LYS:HD2	2:B:401:LYS:N	2.14	0.41
2:B:189:LEU:HD13	2:B:189:LEU:C	2.45	0.41
2:B:209:ALA:O	2:B:210:GLU:C	2.63	0.41
2:B:222:LYS:O	2:B:223:GLY:C	2.63	0.41
2:B:270:PHE:CD2	2:B:270:PHE:C	2.97	0.41
2:B:322:GLU:CD	2:B:322:GLU:N	2.77	0.41
1:A:305:GLY:C	1:A:307:PRO:HD2	2.44	0.41
2:B:5:THR:HG21	2:B:228:GLU:CD	2.44	0.41
2:B:216:SER:O	2:B:217:PHE:C	2.63	0.41
2:B:221:ARG:O	2:B:222:LYS:C	2.62	0.41
2:B:371:GLY:HA2	2:B:374:LYS:HE2	2.01	0.41
1:A:3:ILE:C	1:A:5:TYR:H	2.29	0.41
1:A:64:LYS:O	1:A:66:GLN:HG3	2.20	0.41
1:A:121:LYS:HZ2	1:A:121:LYS:HG3	1.71	0.41
1:A:182:PRO:C	1:A:184:ALA:N	2.77	0.41
1:A:461:ASP:CG	1:A:461:ASP:O	2.61	0.41
2:B:39:VAL:HG23	2:B:40:ILE:N	2.34	0.41
2:B:66:LEU:N	2:B:66:LEU:CD1	2.83	0.41
2:B:246:ARG:HH11	2:B:246:ARG:HG2	1.86	0.41
2:B:390:PHE:O	2:B:391:PRO:C	2.63	0.41
1:A:196:GLY:HA3	3:C:57:LEU:HD11	2.02	0.41
1:A:390:ASP:O	1:A:391:LYS:C	2.64	0.41
2:B:38:ASN:OD1	2:B:40:ILE:N	2.53	0.41
2:B:404:MET:HB3	2:B:410:VAL:HG13	2.02	0.41
3:C:9:VAL:HG11	3:C:25:THR:HG23	2.02	0.41
3:C:33:GLU:OE1	3:C:33:GLU:CA	2.69	0.41
2:B:20:LYS:HD3	2:B:144:GLN:O	2.21	0.41
2:B:135:GLU:O	3:C:93:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:PHE:O	2:B:218:ASN:C	2.62	0.41
1:A:21:LYS:O	1:A:25:VAL:HG23	2.21	0.41
2:B:19:SER:HA	2:B:25:SER:O	2.20	0.41
2:B:157:ILE:CD1	2:B:162:GLU:HB2	2.51	0.41
3:C:51:GLU:HA	3:C:52:PRO:HD3	1.86	0.41
1:A:132:SER:C	1:A:134:GLU:H	2.28	0.41
1:A:262:ALA:O	1:A:264:PRO:HD3	2.20	0.41
1:A:461:ASP:OD2	1:A:464:THR:HB	2.21	0.41
2:B:346:GLY:O	2:B:347:GLY:C	2.62	0.41
2:B:402:GLN:O	2:B:406:ASP:HB2	2.20	0.41
3:C:33:GLU:OE1	3:C:33:GLU:HA	2.21	0.41
1:A:124:MET:CE	1:A:128:ALA:H	2.34	0.41
1:A:188:VAL:CG1	1:A:217:THR:O	2.67	0.41
2:B:6:VAL:HG13	2:B:158:ARG:NH2	2.33	0.41
1:A:166:LEU:O	1:A:167:VAL:CG1	2.69	0.40
1:A:211:ASP:O	1:A:212:GLN:HB2	2.21	0.40
1:A:340:GLU:OE1	1:A:344:LYS:HE3	2.21	0.40
2:B:184:MET:SD	2:B:216:SER:HA	2.61	0.40
1:A:84:THR:HG23	1:A:121:LYS:HE3	1.99	0.40
1:A:222:ASP:O	1:A:223:ASN:C	2.64	0.40
2:B:309:LEU:HG	2:B:310:PRO:N	2.35	0.40
2:B:324:SER:O	2:B:327:PHE:HB3	2.22	0.40
2:B:355:ASN:HD22	2:B:355:ASN:HA	1.60	0.40
2:B:404:MET:HB3	2:B:409:LEU:O	2.22	0.40
1:A:108:MET:CE	1:A:111:LEU:HD12	2.51	0.40
1:A:344:LYS:HB3	3:C:19:GLN:HB2	2.02	0.40
2:B:233:GLU:C	2:B:235:LEU:N	2.78	0.40
2:B:316:VAL:HG11	2:B:345:MET:HG2	2.02	0.40
2:B:402:GLN:CA	2:B:402:GLN:HE21	2.34	0.40
3:C:29:ALA:O	3:C:33:GLU:HB2	2.22	0.40
1:A:257:LYS:CB	1:A:291:GLY:HA3	2.52	0.40
2:B:12:HIS:CE1	2:B:150:GLU:HG3	2.56	0.40
2:B:73:GLU:C	2:B:97:GLN:HE21	2.29	0.40
2:B:276:VAL:HA	2:B:277:PRO:HD3	1.94	0.40
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.71	0.40
1:A:339:LEU:HD11	1:A:343:TYR:CE2	2.54	0.40
1:A:425:ASP:O	1:A:429:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	483/485 (100%)	395 (82%)	70 (14%)	18 (4%)	2	15
2	B	408/483 (84%)	314 (77%)	76 (19%)	18 (4%)	2	12
3	C	96/100 (96%)	73 (76%)	15 (16%)	8 (8%)	0	4
All	All	987/1068 (92%)	782 (79%)	161 (16%)	44 (4%)	2	12

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	242	GLY
2	B	243	GLN
2	B	394	ALA
3	C	22	PRO
3	C	23	GLU
3	C	59	LEU
3	C	97	GLU
1	A	147	HIS
1	A	211	ASP
1	A	335	GLU
1	A	336	ALA
2	B	315	HIS
2	B	347	GLY
3	C	94	ILE
1	A	4	ARG
1	A	80	ASP
1	A	178	SER
2	B	81	TYR
2	B	110	ASP
2	B	200	TYR
1	A	88	GLU
1	A	132	SER
1	A	146	ASP
1	A	212	GLN

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Mol	Chain	Res	Type
1	A	408	ALA
2	B	216	SER
2	B	355	ASN
2	B	398	GLY
1	A	2	SER
1	A	137	TYR
2	B	230	ARG
2	B	322	GLU
3	C	58	ASP
3	C	92	PRO
1	A	29	ILE
1	A	375	TYR
2	B	263	GLY
2	B	410	VAL
3	C	4	VAL
1	A	418	PRO
2	B	316	VAL
1	A	182	PRO
2	B	260	VAL
2	B	296	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	406/406 (100%)	381 (94%)	25 (6%)	16	43
2	B	356/419 (85%)	307 (86%)	49 (14%)	3	14
3	C	86/88 (98%)	70 (81%)	16 (19%)	1	6
All	All	848/913 (93%)	758 (89%)	90 (11%)	6	23

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ARG

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Mol	Chain	Res	Type
1	A	27	LYS
1	A	31	ASP
1	A	52	ILE
1	A	83	ILE
1	A	87	LEU
1	A	118	LEU
1	A	122	LEU
1	A	139	LYS
1	A	143	ASN
1	A	169	LEU
1	A	181	GLN
1	A	206	PHE
1	A	221	LYS
1	A	263	LEU
1	A	268	LEU
1	A	287	LEU
1	A	289	SER
1	A	299	LEU
1	A	302	THR
1	A	349	GLU
1	A	414	GLU
1	A	419	LEU
1	A	433	LEU
2	B	3	PHE
2	B	4	GLU
2	B	5	THR
2	B	23	SER
2	B	28	HIS
2	B	50	VAL
2	B	73	GLU
2	B	84	PRO
2	B	96	ASP
2	B	99	ILE
2	B	108	GLU
2	B	110	ASP
2	B	113	THR
2	B	114	LYS
2	B	119	THR
2	B	135	GLU
2	B	141	LEU
2	B	157	ILE
2	B	158	ARG

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Mol	Chain	Res	Type
2	B	161	LYS
2	B	167	LEU
2	B	185	GLU
2	B	189	LEU
2	B	207	THR
2	B	212	LYS
2	B	220	VAL
2	B	236	LEU
2	B	237	ASN
2	B	241	ILE
2	B	259	ARG
2	B	260	VAL
2	B	270	PHE
2	B	290	GLN
2	B	296	PRO
2	B	298	GLU
2	B	317	LEU
2	B	333	HIS
2	B	350	GLU
2	B	360	LEU
2	B	363	LYS
2	B	368	ASN
2	B	387	LYS
2	B	388	LYS
2	B	392	GLU
2	B	401	LYS
2	B	402	GLN
2	B	404	MET
2	B	409	LEU
2	B	410	VAL
3	C	3	LYS
3	C	8	GLU
3	C	22	PRO
3	C	24	GLU
3	C	26	GLU
3	C	32	LEU
3	C	33	GLU
3	C	57	LEU
3	C	59	LEU
3	C	60	GLN
3	C	65	GLU
3	C	69	ILE

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Mol	Chain	Res	Type
3	C	92	PRO
3	C	94	ILE
3	C	97	GLU
3	C	98	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	85	ASN
1	A	123	ASN
1	A	143	ASN
1	A	181	GLN
1	A	281	GLN
1	A	301	ASN
1	A	332	HIS
1	A	379	GLN
1	A	479	HIS
2	B	34	ASN
2	B	36	ASN
2	B	94	GLN
2	B	97	GLN
2	B	202	GLN
2	B	213	ASN
2	B	290	GLN
2	B	333	HIS
2	B	342	ASN
2	B	355	ASN
2	B	402	GLN
2	B	411	GLN
3	C	41	GLN
3	C	42	ASN
3	C	60	GLN
3	C	61	ASN
3	C	74	GLN
3	C	88	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
5	ADP	B	601	-	28,29,29	1.41	2 (7%)	43,45,45	1.75	7 (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
5	ADP	B	601	-	-	2/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	ADP	PA-O3A	5.27	1.65	1.59
5	B	601	ADP	O4'-C1'	2.04	1.46	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	ADP	C5-C4-N3	-4.98	119.86	126.72
5	B	601	ADP	N3-C2-N1	-4.57	121.67	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	ADP	N3-C4-N9	3.95	133.88	127.17
5	B	601	ADP	C2-N3-C4	3.78	121.05	111.83
5	B	601	ADP	C5-N7-C8	3.41	108.81	103.45
5	B	601	ADP	C4-C5-N7	-2.85	107.32	110.58
5	B	601	ADP	N9-C8-N7	-2.59	110.26	113.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

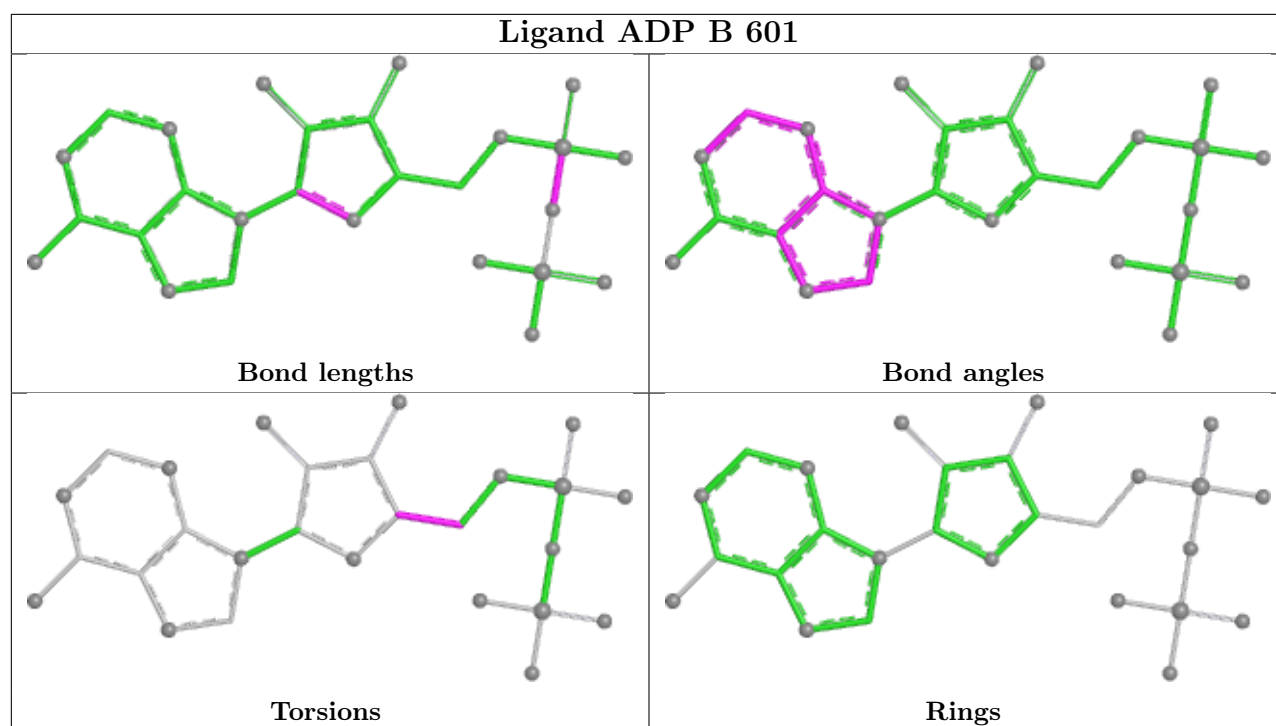
Mol	Chain	Res	Type	Atoms
5	B	601	ADP	O4'-C4'-C5'-O5'
5	B	601	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	ADP	2	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 [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	485/485 (100%)	-0.26	2 (0%) 88 81	24, 24, 40, 60	0
2	B	410/483 (84%)	0.01	5 (1%) 76 63	24, 25, 61, 72	0
3	C	98/100 (98%)	0.10	4 (4%) 41 29	24, 29, 60, 81	0
All	All	993/1068 (92%)	-0.11	11 (1%) 78 65	24, 24, 54, 81	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	8.2
3	C	95	MET	3.3
2	B	411	GLN	3.2
3	C	97	GLU	3.0
2	B	237	ASN	3.0
2	B	240	GLU	2.5
2	B	236	LEU	2.3
3	C	96	ASN	2.3
1	A	2	SER	2.3
3	C	100	ALA	2.1
2	B	241	ILE	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](#)

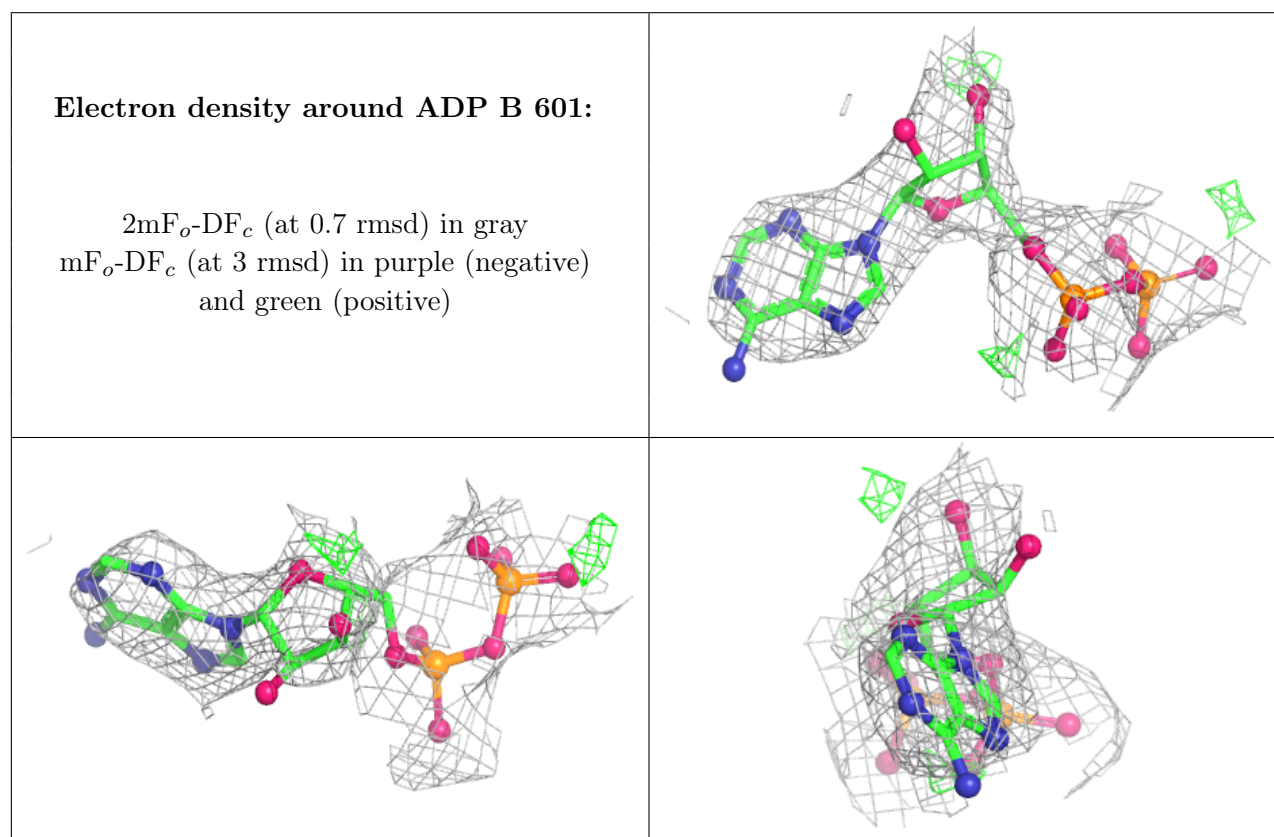
There are no oligosaccharides in this entry.

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	ADP	B	601	27/27	0.82	0.15	28,33,42,43	27
4	MG	B	501	1/1	0.94	0.11	24,24,24,24	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 [i](#)

There are no such residues in this entry.