



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:40 PM UTC

PDB ID : 1Q3Q / pdb_00001q3q
Title : Crystal structure of the chaperonin from Thermococcus strain KS-1 (two-point mutant complexed with AMP-PNP)
Authors : Shomura, Y.; Yoshida, T.; Iizuka, R.; Maruyama, T.; Yohda, M.; Miki, K.
Deposited on : 2003-07-31
Resolution : 2.30 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

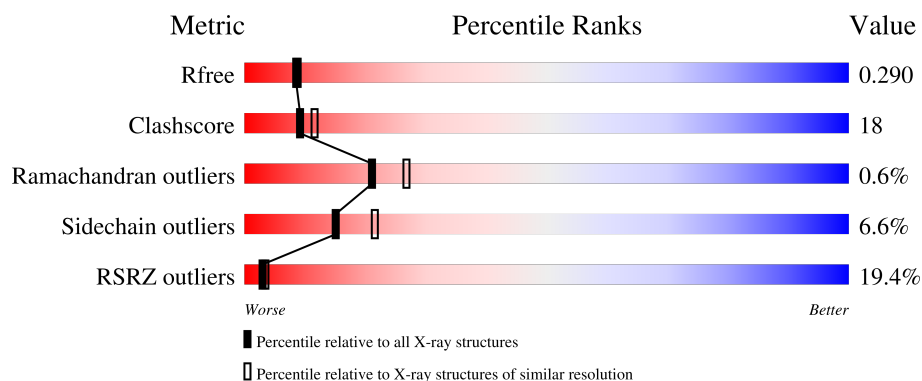
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	548	
1	B	548	
1	C	548	
1	D	548	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16610 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 Thermosome alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3947	2485	673	772	17			
1	B	518	Total	C	N	O	S	0	0	0
			3947	2485	673	772	17			
1	C	518	Total	C	N	O	S	0	0	0
			3947	2485	673	772	17			
1	D	518	Total	C	N	O	S	0	0	0
			3947	2485	673	772	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	CYS	GLY	engineered mutation	UNP O24729
A	125	THR	ILE	engineered mutation	UNP O24729
B	65	CYS	GLY	engineered mutation	UNP O24729
B	125	THR	ILE	engineered mutation	UNP O24729
C	65	CYS	GLY	engineered mutation	UNP O24729
C	125	THR	ILE	engineered mutation	UNP O24729
D	65	CYS	GLY	engineered mutation	UNP O24729
D	125	THR	ILE	engineered mutation	UNP O24729

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

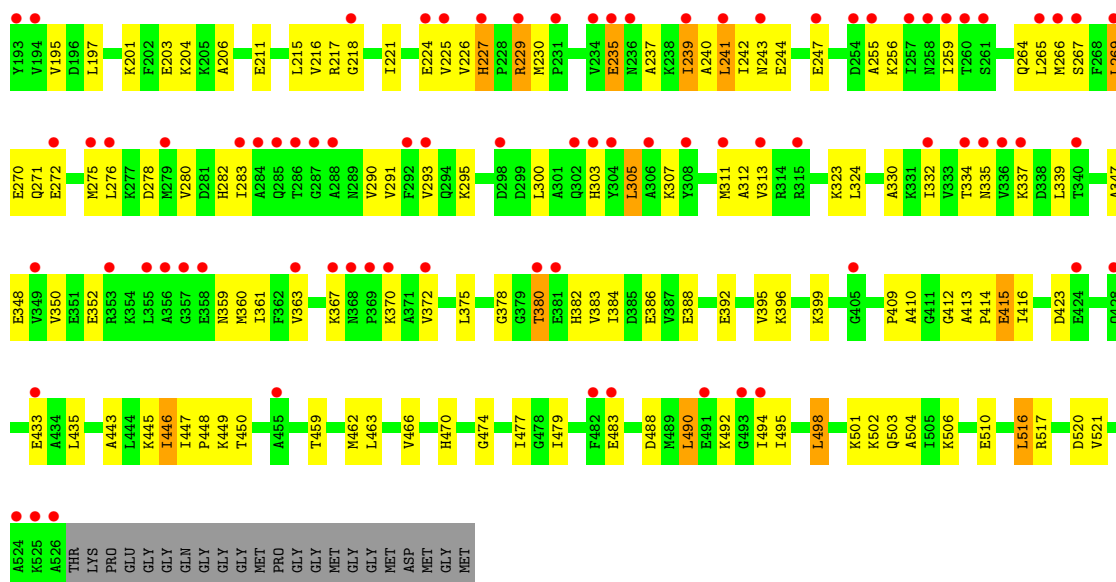
- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



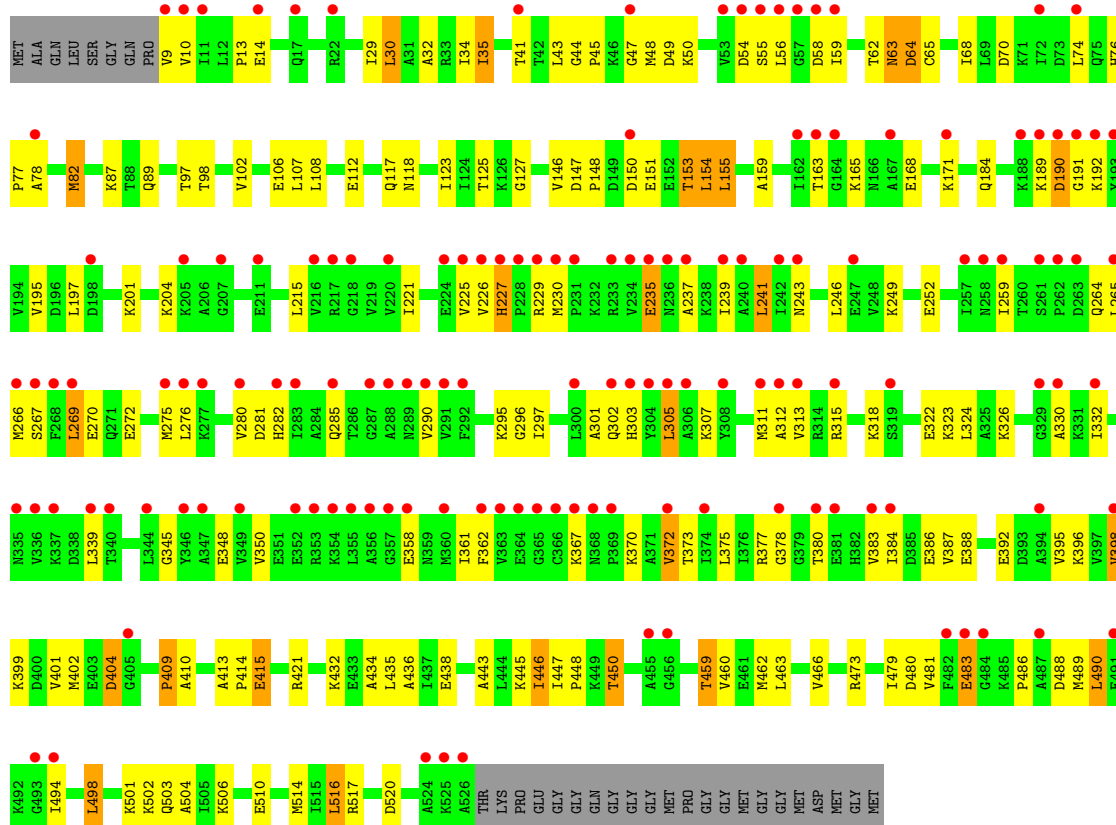
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total	O	0	0
			162	162		
4	B	174	Total	O	0	0
			174	174		
4	C	194	Total	O	0	0
			194	194		
4	D	164	Total	O	0	0
			164	164		

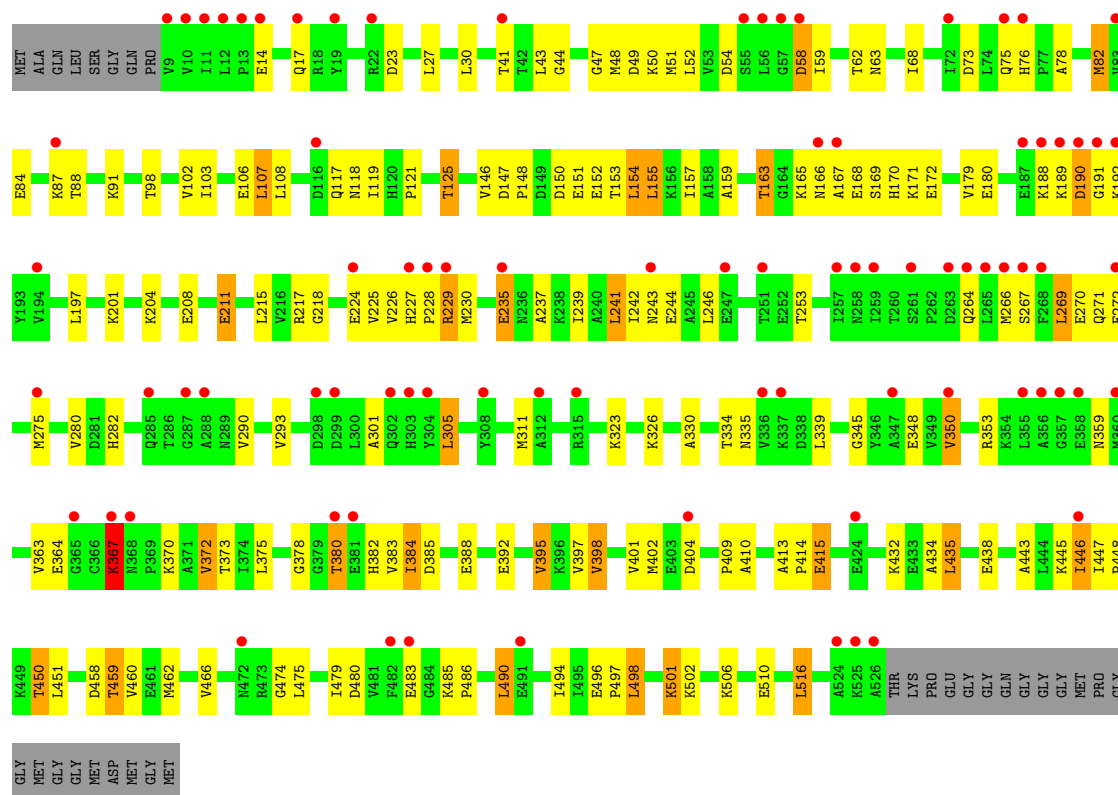


• Molecule 1: Thermosome alpha subunit



• Molecule 1: Thermosome alpha subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	210.83Å 210.83Å 156.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.97 – 2.30 41.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.1 (41.97-2.30) 95.3 (41.97-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.250 0.268 , 0.290	Depositor DCC
R_{free} test set	7449 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.6	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	0.87	EDS
Total number of atoms	16610	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, ANP

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	0/3982	0.94	11/5367 (0.2%)
1	B	0.40	0/3982	0.91	11/5367 (0.2%)
1	C	0.41	0/3982	0.94	18/5367 (0.3%)
1	D	0.42	0/3982	0.93	14/5367 (0.3%)
All	All	0.41	0/15928	0.93	54/21468 (0.3%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	404	ASP	N-CA-C	-8.65	97.65	110.46
1	C	226	VAL	N-CA-C	8.47	119.26	110.62
1	B	226	VAL	N-CA-C	8.41	119.20	110.62
1	B	474	GLY	N-CA-C	8.40	122.46	111.70
1	A	63	ASN	N-CA-C	-8.29	103.61	114.31
1	D	474	GLY	N-CA-C	7.85	124.61	112.45
1	D	168	GLU	N-CA-C	-7.68	103.91	113.28
1	D	226	VAL	N-CA-C	7.33	118.10	110.62
1	B	239	ILE	N-CA-C	6.96	118.60	108.58
1	A	59	ILE	N-CA-C	6.89	117.81	108.17
1	A	226	VAL	N-CA-C	6.88	118.46	110.62
1	A	44	GLY	CA-C-N	6.72	127.26	119.47
1	A	44	GLY	C-N-CA	6.72	127.26	119.47
1	C	63	ASN	N-CA-C	-6.65	105.07	113.72
1	D	239	ILE	N-CA-C	6.59	118.07	108.58
1	A	43	LEU	N-CA-C	6.51	119.72	109.96
1	C	239	ILE	N-CA-C	6.40	117.34	107.99
1	C	225	VAL	N-CA-C	-6.24	101.50	109.30
1	B	225	VAL	N-CA-C	-6.18	100.73	108.89
1	B	227	HIS	CA-C-N	6.13	126.58	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	HIS	C-N-CA	6.13	126.58	119.47
1	D	225	VAL	N-CA-C	-6.12	100.76	108.84
1	C	44	GLY	CA-C-N	6.12	126.57	119.47
1	C	44	GLY	C-N-CA	6.12	126.57	119.47
1	B	59	ILE	N-CA-C	6.06	116.66	108.17
1	A	239	ILE	N-CA-C	6.06	117.30	108.58
1	D	43	LEU	N-CA-C	5.86	118.75	109.96
1	A	474	GLY	N-CA-C	5.84	120.35	112.17
1	C	409	PRO	N-CA-C	-5.75	102.79	111.41
1	C	59	ILE	N-CA-C	5.73	116.74	108.48
1	D	59	ILE	N-CA-C	5.66	116.73	108.53
1	C	64	ASP	N-CA-C	5.61	117.22	109.15
1	D	44	GLY	CA-C-N	5.60	125.44	119.28
1	D	44	GLY	C-N-CA	5.60	125.44	119.28
1	B	44	GLY	CA-C-N	5.57	125.41	119.28
1	B	44	GLY	C-N-CA	5.57	125.41	119.28
1	C	473	ARG	N-CA-C	5.53	119.20	112.23
1	A	225	VAL	N-CA-C	-5.52	102.40	109.30
1	C	252	GLU	N-CA-C	-5.42	105.45	111.36
1	C	43	LEU	N-CA-C	5.40	118.06	109.96
1	D	451	LEU	N-CA-C	-5.29	105.51	111.28
1	B	237	ALA	N-CA-C	5.27	117.87	110.23
1	A	49	ASP	N-CA-C	5.24	117.85	110.14
1	C	237	ALA	N-CA-C	5.21	117.99	110.28
1	C	398	VAL	N-CA-C	-5.19	105.48	110.72
1	D	475	LEU	N-CA-C	5.18	119.91	111.37
1	C	227	HIS	CA-C-N	5.17	125.21	119.32
1	C	227	HIS	C-N-CA	5.17	125.21	119.32
1	D	398	VAL	N-CA-C	-5.14	105.49	110.42
1	D	350	VAL	N-CA-C	-5.12	100.19	107.77
1	A	166	ASN	CA-CB-CG	5.11	117.70	112.60
1	D	237	ALA	N-CA-C	5.09	117.81	110.28
1	C	421	ARG	N-CA-C	5.08	116.90	111.36
1	B	92	GLU	N-CA-C	5.08	117.93	111.69

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	3947	0	4127	158	0
1	B	3947	0	4127	160	0
1	C	3947	0	4127	155	2
1	D	3947	0	4127	155	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	13	2	0
3	B	31	0	13	2	0
3	C	31	0	13	2	0
3	D	31	0	13	2	0
4	A	162	0	0	5	1
4	B	174	0	0	7	2
4	C	194	0	0	6	3
4	D	164	0	0	3	4
All	All	16610	0	16560	591	7

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 18.

All (591) 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:146:VAL:HG23	4:A:1148:HOH:O	1.60	1.01
1:D:272:GLU:HA	1:D:275:MET:HE3	1.45	0.97
1:C:446:ILE:O	1:C:450:THR:HG23	1.65	0.97
1:D:446:ILE:O	1:D:450:THR:HG23	1.65	0.97
1:A:166:ASN:HB3	1:B:517:ARG:HD2	1.48	0.95
1:A:272:GLU:HA	1:A:275:MET:HE3	1.47	0.94
1:D:466:VAL:HG21	1:D:479:ILE:HG12	1.50	0.94
1:C:62:THR:HG22	1:C:64:ASP:H	1.31	0.93
1:C:503:GLN:HE22	1:D:208:GLU:H	1.07	0.93
1:A:462:MET:O	1:A:466:VAL:HG23	1.67	0.93
1:A:163:THR:HG22	1:A:171:LYS:HZ1	1.33	0.91
1:B:271:GLN:HG3	1:B:275:MET:HE2	1.51	0.91
1:C:146:VAL:HG21	1:C:153:THR:HG21	1.51	0.90
1:A:208:GLU:H	1:B:503:GLN:HE22	1.13	0.90
1:A:410:ALA:HB3	1:A:494:ILE:HG22	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:THR:HG22	1:D:383:VAL:H	1.35	0.90
1:C:98:THR:H	3:C:3528:ANP:HNB1	1.20	0.89
1:A:163:THR:HG22	1:A:171:LYS:NZ	1.88	0.88
1:A:271:GLN:HG3	1:A:275:MET:HE2	1.55	0.88
1:C:466:VAL:HG21	1:C:479:ILE:HG12	1.56	0.86
1:B:409:PRO:HB3	1:B:490:LEU:HD13	1.56	0.86
1:A:98:THR:H	3:A:1528:ANP:HNB1	1.23	0.85
1:A:459:THR:HG23	4:C:3189:HOH:O	1.75	0.85
1:B:311:MET:HE1	1:B:350:VAL:CG1	2.07	0.84
1:B:272:GLU:HA	1:B:275:MET:HE3	1.60	0.83
1:B:466:VAL:HG21	1:B:479:ILE:HG12	1.60	0.83
1:D:410:ALA:HB3	1:D:494:ILE:HG22	1.58	0.83
1:C:410:ALA:HB3	1:C:494:ILE:HG22	1.61	0.83
1:B:462:MET:O	1:B:466:VAL:HG23	1.78	0.83
1:D:98:THR:H	3:D:4528:ANP:HNB1	1.27	0.82
1:A:82:MET:HE3	1:A:82:MET:HA	1.61	0.81
1:C:503:GLN:HE22	1:D:208:GLU:N	1.78	0.81
1:B:450:THR:HG22	4:B:2054:HOH:O	1.80	0.80
1:A:166:ASN:HB3	1:B:517:ARG:CD	2.12	0.80
1:B:98:THR:H	3:B:2528:ANP:HNB1	1.30	0.79
1:B:311:MET:HE1	1:B:350:VAL:HG11	1.64	0.79
1:B:170:HIS:CD2	1:B:211:GLU:HG2	2.18	0.79
1:A:409:PRO:HB3	1:A:490:LEU:HD13	1.65	0.78
1:C:503:GLN:NE2	1:D:208:GLU:H	1.79	0.78
1:B:446:ILE:O	1:B:450:THR:HG23	1.83	0.78
1:C:447:ILE:HB	1:C:448:PRO:HD3	1.65	0.78
1:D:82:MET:HE3	1:D:82:MET:HA	1.66	0.77
1:D:235:GLU:O	1:D:348:GLU:O	2.01	0.77
4:C:3074:HOH:O	1:D:380:THR:HG21	1.84	0.77
1:B:211:GLU:HB2	4:B:2030:HOH:O	1.86	0.76
1:B:160:THR:O	1:B:163:THR:HG22	1.85	0.76
1:B:23:ASP:O	1:B:27:LEU:HD23	1.85	0.76
1:C:409:PRO:HB3	1:C:490:LEU:HD13	1.68	0.76
1:A:380:THR:HG21	4:B:1067:HOH:O	1.85	0.75
1:C:275:MET:HE3	1:D:266:MET:HE3	1.68	0.75
1:D:290:VAL:HG13	1:D:311:MET:HE2	1.66	0.75
1:A:466:VAL:HG21	1:A:479:ILE:HG12	1.66	0.75
1:A:266:MET:HE3	1:B:275:MET:SD	2.26	0.74
1:C:462:MET:O	1:C:466:VAL:HG23	1.86	0.74
1:C:204:LYS:HB3	1:C:384:ILE:HG21	1.68	0.74
1:C:204:LYS:HD2	1:C:384:ILE:HG22	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:GLU:HG2	1:A:485:LYS:HE2	1.69	0.74
1:C:62:THR:HG23	1:C:386:GLU:OE2	1.88	0.74
1:D:445:LYS:O	1:D:448:PRO:HD2	1.88	0.74
1:D:170:HIS:CD2	1:D:211:GLU:HG2	2.23	0.74
1:D:311:MET:HE1	1:D:350:VAL:CG1	2.18	0.74
1:B:163:THR:HB	1:B:171:LYS:NZ	2.02	0.73
1:D:434:ALA:O	1:D:438:GLU:HG3	1.89	0.73
1:D:462:MET:O	1:D:466:VAL:HG23	1.87	0.73
1:B:82:MET:HE3	1:B:82:MET:HA	1.69	0.73
1:A:447:ILE:HB	1:A:448:PRO:HD3	1.69	0.73
1:A:150:ASP:OD2	1:A:153:THR:HG23	1.89	0.73
1:D:409:PRO:HB3	1:D:490:LEU:HD13	1.72	0.72
1:B:280:VAL:HG13	1:B:305:LEU:HD13	1.72	0.71
1:B:163:THR:HB	1:B:171:LYS:HZ3	1.53	0.71
1:D:271:GLN:HG3	1:D:275:MET:HE2	1.73	0.71
1:D:189:LYS:HG3	1:D:190:ASP:OD2	1.91	0.71
1:C:280:VAL:HG13	1:C:305:LEU:HD13	1.70	0.71
1:D:23:ASP:O	1:D:27:LEU:HD23	1.90	0.71
1:C:204:LYS:HB3	1:C:384:ILE:CG2	2.21	0.71
1:C:434:ALA:O	1:C:438:GLU:HG3	1.92	0.70
1:A:450:THR:HG22	4:A:1037:HOH:O	1.91	0.70
1:A:415:GLU:HG3	1:A:447:ILE:HB	1.73	0.70
1:C:380:THR:HG23	1:C:383:VAL:H	1.55	0.70
1:A:54:ASP:OD2	1:A:58:ASP:HB3	1.90	0.69
1:A:204:LYS:HB3	1:A:384:ILE:HG21	1.74	0.69
1:B:290:VAL:HG13	1:B:311:MET:HE2	1.73	0.69
1:A:189:LYS:HG2	1:A:192:LYS:O	1.93	0.69
1:C:415:GLU:HG3	1:C:447:ILE:HB	1.74	0.69
1:C:466:VAL:HG22	1:C:486:PRO:HG3	1.73	0.69
1:A:75:GLN:NE2	1:B:13:PRO:HG3	2.07	0.69
1:B:447:ILE:HB	1:B:448:PRO:HD3	1.75	0.69
1:C:54:ASP:OD2	1:C:58:ASP:HB2	1.92	0.69
1:A:443:ALA:O	1:A:446:ILE:HG13	1.93	0.68
1:B:201:LYS:HB2	1:B:323:LYS:HE2	1.76	0.68
1:B:215:LEU:HD21	1:B:372:VAL:HG21	1.76	0.68
1:B:443:ALA:O	1:B:446:ILE:HG13	1.93	0.68
1:A:208:GLU:N	1:B:503:GLN:HE22	1.90	0.68
1:C:32:ALA:HB1	1:C:82:MET:HE2	1.75	0.67
1:B:227:HIS:CE1	1:B:229:ARG:HB2	2.29	0.67
1:A:23:ASP:O	1:A:27:LEU:HD23	1.93	0.67
1:A:50:LYS:HG2	1:B:520:ASP:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:THR:HG22	1:C:383:VAL:HG23	1.76	0.67
1:B:47:GLY:O	1:B:48:MET:HE2	1.94	0.67
1:B:50:LYS:HD2	1:B:68:ILE:HD13	1.77	0.67
1:D:190:ASP:C	1:D:192:LYS:H	2.00	0.67
1:A:459:THR:CG2	4:C:3189:HOH:O	2.40	0.67
1:D:166:ASN:O	1:D:167:ALA:HB3	1.94	0.66
1:B:410:ALA:HB3	1:B:494:ILE:HG22	1.76	0.66
1:B:204:LYS:HB2	1:B:384:ILE:HG21	1.77	0.66
1:D:466:VAL:HG21	1:D:479:ILE:CG1	2.24	0.66
1:A:227:HIS:HD2	1:A:229:ARG:H	1.43	0.66
1:C:401:VAL:O	1:C:404:ASP:O	2.14	0.66
1:D:50:LYS:HD2	1:D:68:ILE:HD13	1.78	0.66
1:C:201:LYS:HB2	1:C:323:LYS:HE2	1.78	0.66
1:A:125:THR:HG21	4:A:1087:HOH:O	1.95	0.65
1:B:311:MET:HE1	1:B:350:VAL:HG12	1.77	0.65
1:B:54:ASP:OD2	1:B:58:ASP:HB3	1.97	0.65
1:B:466:VAL:HG21	1:B:479:ILE:CG1	2.25	0.65
1:C:443:ALA:O	1:C:446:ILE:HG13	1.96	0.65
1:B:243:ASN:O	1:B:295:LYS:HG2	1.97	0.65
1:C:150:ASP:HB3	1:C:153:THR:HG23	1.79	0.65
1:B:266:MET:O	1:B:270:GLU:HG3	1.95	0.64
1:A:208:GLU:H	1:B:503:GLN:NE2	1.92	0.64
1:B:227:HIS:HB3	1:B:230:MET:HG3	1.79	0.64
1:A:82:MET:HA	1:A:82:MET:CE	2.28	0.64
1:C:445:LYS:O	1:C:448:PRO:HD2	1.97	0.64
1:D:146:VAL:HG21	1:D:153:THR:HG21	1.78	0.64
1:D:311:MET:HE1	1:D:350:VAL:HG12	1.78	0.64
1:B:247:GLU:HA	1:B:276:LEU:HD21	1.79	0.64
1:D:498:LEU:HD22	1:D:502:LYS:HG3	1.79	0.64
1:A:335:ASN:OD1	1:A:337:LYS:HG2	1.97	0.64
1:D:447:ILE:HB	1:D:448:PRO:HD3	1.78	0.64
1:C:159:ALA:O	1:C:163:THR:HG23	1.99	0.63
1:B:241:LEU:HB3	1:B:332:ILE:HD13	1.80	0.63
1:D:266:MET:HE2	1:D:266:MET:HA	1.80	0.63
1:B:204:LYS:HB2	1:B:384:ILE:CG2	2.28	0.63
1:C:215:LEU:HD11	1:C:372:VAL:HG13	1.80	0.63
1:A:243:ASN:OD1	1:A:334:THR:HA	1.97	0.63
1:A:189:LYS:HG3	1:A:190:ASP:OD2	1.99	0.63
1:A:244:GLU:HB3	1:A:334:THR:O	1.99	0.63
1:A:410:ALA:HB1	3:A:1528:ANP:O2'	1.99	0.63
1:C:197:LEU:HD22	1:C:395:VAL:CG1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LYS:HD2	1:A:68:ILE:HD13	1.81	0.62
1:D:49:ASP:OD1	1:D:63:ASN:HB2	1.99	0.62
1:A:155:LEU:HD12	1:A:179:VAL:HG21	1.81	0.62
1:C:191:GLY:C	1:C:192:LYS:HD2	2.25	0.62
1:C:410:ALA:HB1	3:C:3528:ANP:O2'	1.98	0.62
1:A:125:THR:HG23	1:A:513:ILE:HG23	1.80	0.62
1:B:241:LEU:HD22	1:B:330:ALA:HB3	1.81	0.62
1:C:32:ALA:HB1	1:C:82:MET:CE	2.29	0.62
1:D:150:ASP:OD1	1:D:153:THR:HG23	1.98	0.62
1:D:415:GLU:HG3	1:D:447:ILE:HB	1.80	0.62
1:A:276:LEU:HD23	1:A:300:LEU:HB3	1.81	0.62
1:C:215:LEU:HD11	1:C:372:VAL:CG1	2.29	0.62
1:A:197:LEU:HD22	1:A:395:VAL:CG1	2.30	0.61
1:A:446:ILE:O	1:A:450:THR:HG23	2.00	0.61
1:C:108:LEU:HD23	1:C:516:LEU:HD22	1.82	0.61
1:C:259:ILE:HD13	1:C:265:LEU:HD23	1.83	0.61
1:D:47:GLY:O	1:D:48:MET:HE2	2.01	0.61
1:A:146:VAL:CG2	4:A:1148:HOH:O	2.31	0.61
1:C:498:LEU:HD22	1:C:502:LYS:HG3	1.82	0.61
1:D:241:LEU:HD22	1:D:330:ALA:HB3	1.83	0.61
1:B:433:GLU:H	1:B:433:GLU:CD	2.09	0.61
1:A:204:LYS:HB3	1:A:384:ILE:CG2	2.30	0.61
1:B:215:LEU:HD21	1:B:372:VAL:CG2	2.31	0.60
1:D:462:MET:HE2	1:D:479:ILE:HG23	1.82	0.60
1:A:227:HIS:CD2	1:A:229:ARG:H	2.18	0.60
1:D:87:LYS:HE2	1:D:87:LYS:HA	1.82	0.60
1:D:76:HIS:HD2	1:D:78:ALA:H	1.48	0.60
1:B:215:LEU:HD23	1:B:216:VAL:N	2.16	0.60
1:D:443:ALA:O	1:D:446:ILE:HG13	2.01	0.60
1:B:278:ASP:OD2	4:B:2073:HOH:O	2.17	0.60
1:A:170:HIS:CD2	1:A:211:GLU:HG2	2.37	0.59
1:D:155:LEU:HD12	1:D:179:VAL:HG21	1.84	0.59
1:D:76:HIS:CD2	1:D:78:ALA:H	2.20	0.59
1:A:380:THR:HG23	1:A:383:VAL:H	1.68	0.59
1:A:146:VAL:HG22	1:A:147:ASP:N	2.17	0.59
1:C:56:LEU:N	1:C:56:LEU:HD12	2.17	0.59
1:D:378:GLY:N	1:D:384:ILE:HD11	2.17	0.59
1:D:410:ALA:HB1	3:D:4528:ANP:O2'	2.03	0.59
1:A:47:GLY:O	1:A:48:MET:HE2	2.03	0.59
1:C:62:THR:HG22	1:C:63:ASN:H	1.67	0.59
1:D:311:MET:HE1	1:D:350:VAL:HG11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:LYS:C	1:D:448:PRO:HD2	2.27	0.58
1:D:201:LYS:HB2	1:D:323:LYS:HE2	1.85	0.58
1:B:206:ALA:HA	1:B:384:ILE:HD12	1.84	0.58
1:A:170:HIS:NE2	1:A:211:GLU:HG2	2.18	0.58
1:A:227:HIS:CD2	1:A:229:ARG:HB2	2.38	0.58
1:A:239:ILE:N	1:A:239:ILE:HD12	2.19	0.58
1:C:108:LEU:HD23	1:C:516:LEU:CD2	2.33	0.58
1:C:13:PRO:HG3	1:D:75:GLN:NE2	2.19	0.57
1:C:70:ASP:HB2	1:C:87:LYS:HE2	1.86	0.57
1:A:266:MET:HE2	1:A:269:LEU:HD23	1.85	0.57
1:C:266:MET:O	1:C:270:GLU:HG3	2.04	0.57
1:A:204:LYS:HD2	1:A:384:ILE:HG22	1.86	0.57
1:B:466:VAL:CG2	1:B:479:ILE:HG12	2.34	0.57
1:C:108:LEU:CD2	1:C:516:LEU:HD22	2.35	0.57
1:D:244:GLU:HB2	1:D:334:THR:O	2.03	0.57
1:B:244:GLU:HB3	1:B:334:THR:O	2.04	0.57
1:C:62:THR:HG22	1:C:63:ASN:N	2.19	0.57
1:A:282:HIS:HE1	1:A:339:LEU:O	1.88	0.57
1:B:445:LYS:O	1:B:448:PRO:HD2	2.04	0.57
1:D:483:GLU:HG3	1:D:485:LYS:HE3	1.85	0.57
1:D:159:ALA:O	1:D:163:THR:HG22	2.05	0.56
1:B:87:LYS:O	1:B:91:LYS:HG2	2.05	0.56
1:A:148:PRO:O	1:A:402:MET:HG2	2.06	0.56
1:A:380:THR:HG22	1:A:383:VAL:HB	1.87	0.56
1:B:151:GLU:HG2	1:B:155:LEU:HD22	1.87	0.56
1:A:117:GLN:O	1:A:118:ASN:HB2	2.06	0.56
1:C:380:THR:HG22	1:C:383:VAL:CG2	2.36	0.56
1:D:146:VAL:HG22	1:D:147:ASP:N	2.20	0.56
1:A:513:ILE:O	1:A:517:ARG:HG3	2.06	0.56
1:A:434:ALA:O	1:A:438:GLU:HG3	2.06	0.55
1:D:266:MET:O	1:D:270:GLU:HG3	2.05	0.55
1:D:413:ALA:HB3	1:D:414:PRO:HD3	1.88	0.55
1:B:230:MET:HE2	1:B:305:LEU:HB3	1.89	0.55
1:B:224:GLU:HG2	1:B:359:ASN:HB2	1.88	0.55
1:A:146:VAL:HG21	1:A:153:THR:HG21	1.87	0.55
1:C:227:HIS:CD2	1:C:229:ARG:H	2.24	0.55
1:C:266:MET:HE2	1:C:266:MET:HA	1.88	0.55
1:B:189:LYS:HG3	1:B:190:ASP:OD2	2.07	0.55
1:C:201:LYS:HB2	1:C:323:LYS:CE	2.36	0.55
1:C:380:THR:CG2	1:C:383:VAL:HG23	2.37	0.55
1:B:498:LEU:HD22	1:B:502:LYS:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:MET:HE3	1:D:266:MET:CE	2.35	0.55
1:C:30:LEU:HD22	1:C:34:ILE:HD11	1.89	0.55
1:A:264:GLN:HA	1:A:267:SER:OG	2.07	0.54
1:C:313:VAL:HG21	1:C:361:ILE:CD1	2.36	0.54
1:B:415:GLU:HG3	1:B:447:ILE:HB	1.89	0.54
1:C:227:HIS:HB3	1:C:230:MET:HG3	1.88	0.54
1:B:190:ASP:C	1:B:192:LYS:H	2.16	0.54
1:C:47:GLY:O	1:C:48:MET:HE2	2.07	0.54
1:A:146:VAL:HG22	1:A:147:ASP:H	1.72	0.54
1:B:335:ASN:HB3	1:B:337:LYS:HG2	1.89	0.54
1:A:211:GLU:HB2	4:A:1110:HOH:O	2.07	0.54
1:C:462:MET:HE2	1:C:479:ILE:HG23	1.89	0.54
1:B:37:GLU:HA	1:B:40:ARG:HG2	1.90	0.54
1:B:150:ASP:OD1	1:B:153:THR:HG23	2.08	0.54
1:C:281:ASP:O	1:C:285:GLN:HG3	2.08	0.54
1:B:410:ALA:HB1	3:B:2528:ANP:O2'	2.07	0.54
1:C:311:MET:HE1	1:C:350:VAL:CG1	2.38	0.54
1:C:77:PRO:HB2	1:D:51:MET:CE	2.37	0.53
1:A:206:ALA:HA	1:A:384:ILE:HD12	1.90	0.53
1:C:517:ARG:NH1	1:D:165:LYS:HA	2.24	0.53
1:D:180:GLU:CD	1:D:215:LEU:HD23	2.33	0.53
1:A:241:LEU:HD23	1:A:332:ILE:HD13	1.90	0.53
1:B:264:GLN:HA	1:B:267:SER:OG	2.08	0.53
1:B:388:GLU:O	1:B:392:GLU:HG3	2.09	0.53
1:D:415:GLU:H	1:D:415:GLU:CD	2.16	0.53
1:B:155:LEU:HD13	1:B:179:VAL:HG21	1.89	0.53
1:C:76:HIS:CD2	1:C:78:ALA:H	2.27	0.53
1:C:89:GLN:HE22	1:C:504:ALA:N	2.07	0.53
1:B:449:LYS:HG3	1:B:459:THR:CG2	2.39	0.53
1:C:241:LEU:HD23	1:C:332:ILE:HD13	1.89	0.53
1:D:372:VAL:HG13	1:D:373:THR:N	2.23	0.53
1:A:483:GLU:CG	1:A:485:LYS:HE2	2.39	0.52
1:C:282:HIS:HE1	1:C:339:LEU:O	1.91	0.52
1:D:280:VAL:HG13	1:D:305:LEU:HD13	1.91	0.52
1:A:201:LYS:HB2	1:A:323:LYS:HE2	1.92	0.52
1:C:517:ARG:NH1	1:D:166:ASN:H	2.07	0.52
1:B:216:VAL:O	1:B:372:VAL:HG22	2.09	0.52
1:B:380:THR:HG22	1:B:383:VAL:H	1.74	0.52
1:D:106:GLU:HB2	1:D:446:ILE:HG12	1.91	0.52
1:D:496:GLU:HG3	4:D:4061:HOH:O	2.09	0.52
1:B:409:PRO:HB3	1:B:490:LEU:CD1	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:THR:HG22	1:A:383:VAL:CG2	2.40	0.52
1:B:380:THR:HG22	1:B:382:HIS:N	2.24	0.52
1:C:326:LYS:HB3	1:C:370:LYS:HB2	1.90	0.52
1:B:144:ILE:HD11	1:B:490:LEU:HD21	1.92	0.52
1:D:155:LEU:CD1	1:D:179:VAL:HG21	2.40	0.52
1:D:215:LEU:HD11	1:D:372:VAL:CG1	2.40	0.52
1:B:265:LEU:O	1:B:269:LEU:HD22	2.09	0.52
1:C:409:PRO:HB3	1:C:490:LEU:CD1	2.38	0.52
1:C:190:ASP:C	1:C:192:LYS:H	2.18	0.52
1:D:91:LYS:HB2	1:D:91:LYS:HZ2	1.74	0.52
1:A:445:LYS:O	1:A:448:PRO:HD2	2.10	0.51
1:C:117:GLN:O	1:C:118:ASN:HB2	2.08	0.51
1:C:195:VAL:HB	1:C:399:LYS:HG3	1.91	0.51
1:D:388:GLU:O	1:D:392:GLU:HG3	2.10	0.51
1:A:239:ILE:HG22	1:A:241:LEU:HD13	1.92	0.51
1:A:230:MET:HE2	1:A:305:LEU:HB3	1.92	0.51
1:A:380:THR:CG2	1:A:383:VAL:H	2.22	0.51
1:A:235:GLU:O	1:A:348:GLU:O	2.28	0.51
1:B:188:LYS:NZ	1:B:191:GLY:H	2.07	0.51
1:D:41:THR:O	1:D:41:THR:HG22	2.09	0.51
1:D:190:ASP:C	1:D:192:LYS:N	2.68	0.51
1:D:242:ILE:O	1:D:293:VAL:HA	2.11	0.51
1:C:146:VAL:HG22	1:C:147:ASP:N	2.24	0.51
1:D:353:ARG:HH22	1:D:364:GLU:CD	2.17	0.51
1:A:227:HIS:HB3	1:A:230:MET:HG3	1.91	0.51
1:B:146:VAL:HG21	1:B:153:THR:HG21	1.91	0.51
1:D:154:LEU:HG	1:D:398:VAL:HG13	1.93	0.51
1:B:68:ILE:O	1:B:72:ILE:HG13	2.11	0.51
1:C:55:SER:OG	1:C:56:LEU:HD12	2.11	0.51
1:B:106:GLU:CB	1:B:446:ILE:HG12	2.41	0.51
1:D:204:LYS:HD2	1:D:384:ILE:HG23	1.92	0.51
1:A:144:ILE:HD11	1:A:490:LEU:HD21	1.93	0.50
1:A:258:ASN:HD22	1:A:258:ASN:N	2.08	0.50
1:A:259:ILE:HD13	1:A:265:LEU:HD23	1.93	0.50
1:B:182:VAL:CG2	1:B:395:VAL:HG13	2.42	0.50
1:C:297:ILE:HG22	1:C:302:GLN:HG3	1.93	0.50
1:C:517:ARG:HD2	1:D:166:ASN:HB3	1.93	0.50
1:B:282:HIS:HE1	1:B:339:LEU:O	1.94	0.50
1:C:41:THR:HG22	1:C:41:THR:O	2.12	0.50
1:C:301:ALA:O	1:C:305:LEU:HD22	2.12	0.50
1:C:517:ARG:HH12	1:D:165:LYS:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:LYS:HD2	1:D:384:ILE:CG2	2.41	0.50
1:A:297:ILE:HG22	1:A:302:GLN:HG3	1.92	0.50
1:B:462:MET:HE2	1:B:479:ILE:HG23	1.93	0.50
1:D:82:MET:HA	1:D:82:MET:CE	2.39	0.50
1:D:334:THR:HG22	1:D:335:ASN:ND2	2.25	0.50
1:B:157:ILE:HD13	1:B:495:ILE:HG13	1.92	0.50
1:B:215:LEU:HD23	1:B:215:LEU:C	2.37	0.50
1:C:150:ASP:OD1	1:C:153:THR:HG22	2.12	0.50
1:D:146:VAL:HG22	1:D:147:ASP:H	1.77	0.50
1:B:117:GLN:O	1:B:118:ASN:HB2	2.11	0.50
1:C:150:ASP:HB3	1:C:153:THR:CG2	2.41	0.50
1:B:413:ALA:HB3	1:B:414:PRO:HD3	1.94	0.50
1:C:56:LEU:HD12	1:C:56:LEU:H	1.75	0.50
1:C:163:THR:HG22	1:C:171:LYS:HD3	1.94	0.50
1:C:290:VAL:HG13	1:C:311:MET:HE2	1.93	0.50
1:C:378:GLY:N	1:C:384:ILE:HD11	2.27	0.50
1:C:410:ALA:O	1:C:489:MET:HG3	2.12	0.50
1:C:480:ASP:OD1	1:C:483:GLU:HB2	2.11	0.49
1:A:218:GLY:HA3	1:A:363:VAL:O	2.12	0.49
1:B:76:HIS:HD2	1:B:78:ALA:H	1.58	0.49
1:A:466:VAL:HG21	1:A:479:ILE:CG1	2.39	0.49
1:C:13:PRO:HD3	1:D:73:ASP:O	2.12	0.49
1:C:313:VAL:HG21	1:C:361:ILE:HD12	1.93	0.49
1:B:488:ASP:O	1:B:492:LYS:HG2	2.12	0.49
1:A:35:ILE:HD11	1:A:74:LEU:HD22	1.94	0.49
1:B:9:VAL:O	1:B:11:ILE:HG12	2.12	0.49
1:B:242:ILE:O	1:B:293:VAL:HA	2.12	0.49
1:B:259:ILE:HD13	1:B:265:LEU:HD23	1.93	0.49
1:D:188:LYS:HE3	1:D:191:GLY:HA2	1.94	0.49
1:D:119:ILE:HD11	1:D:435:LEU:HD23	1.95	0.49
1:D:165:LYS:O	1:D:166:ASN:C	2.53	0.49
1:A:73:ASP:O	1:B:13:PRO:HD3	2.12	0.49
1:A:206:ALA:HA	1:A:384:ILE:CD1	2.41	0.49
1:D:266:MET:CE	1:D:269:LEU:HD23	2.42	0.49
1:D:466:VAL:HG22	1:D:486:PRO:HG3	1.94	0.49
1:A:224:GLU:HG2	1:A:359:ASN:HB2	1.95	0.48
1:B:197:LEU:HD22	1:B:395:VAL:HG12	1.95	0.48
1:D:197:LEU:HD22	1:D:395:VAL:CG1	2.42	0.48
1:A:330:ALA:HB2	1:A:345:GLY:HA3	1.94	0.48
1:D:506:LYS:O	1:D:510:GLU:HG3	2.14	0.48
1:C:259:ILE:CD1	1:C:265:LEU:HD23	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ALA:HB2	1:C:345:GLY:HA3	1.95	0.48
1:D:224:GLU:HG2	1:D:359:ASN:HB2	1.96	0.48
1:B:412:GLY:O	1:B:415:GLU:HG2	2.13	0.48
1:C:215:LEU:CD1	1:C:372:VAL:HG13	2.42	0.48
1:C:388:GLU:O	1:C:392:GLU:HG3	2.13	0.48
1:D:218:GLY:HA3	1:D:363:VAL:O	2.13	0.48
1:D:119:ILE:CD1	1:D:435:LEU:HD23	2.43	0.48
1:D:157:ILE:HG13	1:D:401:VAL:HG21	1.96	0.48
1:A:9:VAL:HG13	1:A:9:VAL:O	2.12	0.48
1:C:517:ARG:CD	1:D:166:ASN:HB3	2.43	0.48
1:A:410:ALA:HB2	1:A:496:GLU:HG2	1.96	0.48
1:B:449:LYS:HG3	1:B:459:THR:HG23	1.96	0.48
1:C:76:HIS:HD2	1:C:78:ALA:H	1.60	0.48
1:B:201:LYS:HB2	1:B:323:LYS:CE	2.43	0.48
1:C:106:GLU:HB2	1:C:446:ILE:HG12	1.95	0.48
1:C:230:MET:HE1	1:C:312:ALA:HB3	1.94	0.48
1:A:62:THR:HG23	1:A:389:ARG:NE	2.28	0.48
1:C:9:VAL:HG13	1:C:9:VAL:O	2.14	0.47
1:D:166:ASN:O	1:D:167:ALA:CB	2.60	0.47
1:A:413:ALA:HB3	1:A:414:PRO:HD3	1.96	0.47
1:C:311:MET:HE1	1:C:350:VAL:HG12	1.96	0.47
1:D:103:ILE:HG22	1:D:107:LEU:HD22	1.95	0.47
1:C:30:LEU:HD22	1:C:34:ILE:CD1	2.44	0.47
1:A:157:ILE:HG13	1:A:401:VAL:HG21	1.95	0.47
1:A:380:THR:HG22	1:A:383:VAL:CB	2.44	0.47
1:B:49:ASP:OD1	1:B:63:ASN:HB2	2.13	0.47
1:B:224:GLU:HG2	1:B:359:ASN:CB	2.45	0.47
1:C:517:ARG:HH11	1:D:166:ASN:H	1.62	0.47
1:D:121:PRO:O	1:D:125:THR:HB	2.15	0.47
1:D:264:GLN:HA	1:D:267:SER:OG	2.14	0.47
1:B:89:GLN:HE22	1:B:504:ALA:N	2.13	0.47
1:C:377:ARG:C	1:C:384:ILE:HD11	2.39	0.47
1:A:76:HIS:CD2	1:A:78:ALA:H	2.33	0.47
1:B:95:ASP:OD1	1:B:161:SER:CB	2.63	0.47
1:B:266:MET:HE2	1:B:269:LEU:HD23	1.97	0.47
1:B:303:HIS:CE1	1:B:307:LYS:HD2	2.50	0.47
1:C:148:PRO:O	1:C:402:MET:HG2	2.15	0.47
1:C:517:ARG:NH1	1:D:166:ASN:N	2.63	0.47
1:D:380:THR:HG23	1:D:382:HIS:H	1.80	0.47
1:D:432:LYS:O	1:D:435:LEU:HB2	2.15	0.47
1:A:62:THR:CG2	1:A:389:ARG:NE	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:THR:HG22	1:A:383:VAL:HG23	1.96	0.47
1:C:264:GLN:HA	1:C:267:SER:OG	2.15	0.47
1:D:204:LYS:HB3	1:D:384:ILE:CG2	2.45	0.47
1:C:350:VAL:HA	1:C:362:PHE:O	2.15	0.47
1:D:215:LEU:HD11	1:D:372:VAL:HG11	1.96	0.47
1:A:273:GLU:OE2	1:B:337:LYS:HE2	2.14	0.46
1:A:506:LYS:O	1:A:510:GLU:HG3	2.15	0.46
1:D:301:ALA:O	1:D:305:LEU:HD22	2.15	0.46
1:A:272:GLU:CA	1:A:275:MET:HE3	2.32	0.46
1:A:89:GLN:HE22	1:A:504:ALA:N	2.13	0.46
1:B:82:MET:HA	1:B:82:MET:CE	2.41	0.46
1:C:506:LYS:O	1:C:510:GLU:HG3	2.16	0.46
1:D:151:GLU:HG2	1:D:155:LEU:HD22	1.98	0.46
1:B:9:VAL:O	1:B:9:VAL:HG13	2.14	0.46
1:B:188:LYS:HZ3	1:B:191:GLY:H	1.62	0.46
1:C:192:LYS:HD2	1:C:192:LYS:N	2.29	0.46
1:A:75:GLN:HE21	1:B:13:PRO:HG3	1.77	0.46
1:A:498:LEU:HD22	1:A:502:LYS:HG3	1.98	0.46
1:C:221:ILE:HD11	1:C:324:LEU:HD11	1.97	0.46
1:D:117:GLN:O	1:D:118:ASN:HB2	2.15	0.46
1:B:206:ALA:HA	1:B:384:ILE:CD1	2.46	0.46
1:C:445:LYS:C	1:C:448:PRO:HD2	2.40	0.46
1:D:227:HIS:CD2	1:D:229:ARG:H	2.33	0.46
1:D:326:LYS:HB3	1:D:370:LYS:HB2	1.98	0.46
1:A:82:MET:HE3	1:A:82:MET:CA	2.40	0.46
1:B:221:ILE:HD11	1:B:324:LEU:HD11	1.98	0.46
1:B:239:ILE:HD11	1:B:347:ALA:CB	2.46	0.46
1:A:204:LYS:HD3	1:A:388:GLU:OE2	2.15	0.46
1:B:106:GLU:HB2	1:B:446:ILE:HG12	1.96	0.46
1:C:227:HIS:CD2	1:C:229:ARG:HB2	2.51	0.46
1:C:488:ASP:OD1	1:C:490:LEU:HB2	2.15	0.46
1:D:227:HIS:HD2	1:D:229:ARG:H	1.63	0.46
1:D:272:GLU:CA	1:D:275:MET:HE3	2.32	0.46
1:C:35:ILE:HD13	1:C:35:ILE:HA	1.85	0.45
1:C:45:PRO:HB2	1:C:481:VAL:HG21	1.97	0.45
1:C:65:CYS:HB3	1:C:97:THR:OG1	2.16	0.45
1:C:358:GLU:HB3	4:C:3188:HOH:O	2.15	0.45
1:C:303:HIS:O	1:C:307:LYS:HG3	2.16	0.45
1:D:76:HIS:HD2	1:D:78:ALA:N	2.13	0.45
1:D:466:VAL:CG2	1:D:479:ILE:HG12	2.35	0.45
1:D:372:VAL:CG1	1:D:373:THR:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:MET:CE	1:B:77:PRO:HB2	2.46	0.45
1:B:76:HIS:CD2	1:B:78:ALA:H	2.34	0.45
1:C:275:MET:CE	1:D:266:MET:HE3	2.43	0.45
1:C:380:THR:O	1:C:384:ILE:HG12	2.15	0.45
1:D:54:ASP:OD2	1:D:58:ASP:HB2	2.16	0.45
1:C:189:LYS:HG3	1:C:190:ASP:OD2	2.16	0.45
1:B:235:GLU:O	1:B:348:GLU:O	2.35	0.45
1:C:318:LYS:O	1:C:322:GLU:HG3	2.16	0.45
1:D:98:THR:O	1:D:102:VAL:HG23	2.17	0.45
1:C:249:LYS:HB2	1:D:269:LEU:HD21	1.99	0.45
1:D:106:GLU:CB	1:D:446:ILE:HG12	2.47	0.45
1:D:243:ASN:OD1	1:D:334:THR:HA	2.17	0.45
1:A:215:LEU:HD11	1:A:372:VAL:CG1	2.47	0.45
1:A:378:GLY:N	1:A:384:ILE:HD11	2.33	0.45
1:B:197:LEU:HD22	1:B:395:VAL:CG1	2.47	0.44
1:B:240:ALA:HB3	1:B:291:VAL:HG22	1.98	0.44
1:D:217:ARG:NH2	4:D:4002:HOH:O	2.45	0.44
1:A:243:ASN:O	1:A:295:LYS:HG2	2.17	0.44
1:B:180:GLU:HB3	1:B:215:LEU:HD12	1.99	0.44
1:A:159:ALA:O	1:A:163:THR:HG23	2.17	0.44
1:A:273:GLU:CD	1:B:337:LYS:HE2	2.42	0.44
1:C:396:LYS:HE3	4:C:3119:HOH:O	2.17	0.44
1:C:520:ASP:HB3	1:D:50:LYS:HG2	1.98	0.44
1:B:204:LYS:HD2	1:B:384:ILE:HG22	1.98	0.44
1:B:215:LEU:C	1:B:215:LEU:CD2	2.91	0.44
1:C:154:LEU:HG	1:C:398:VAL:HG13	1.99	0.44
1:D:330:ALA:HB2	1:D:345:GLY:HA3	1.99	0.44
1:A:244:GLU:CB	1:A:334:THR:O	2.65	0.44
1:A:256:LYS:HE2	1:B:256:LYS:HB2	1.99	0.44
1:B:386:GLU:HA	1:B:386:GLU:OE2	2.17	0.44
1:B:415:GLU:CD	1:B:415:GLU:H	2.24	0.44
1:C:235:GLU:O	1:C:348:GLU:O	2.36	0.44
1:C:459:THR:HG22	1:C:460:VAL:N	2.32	0.44
1:B:14:GLU:O	1:B:14:GLU:HG3	2.18	0.44
1:C:50:LYS:HD2	1:C:68:ILE:HD13	2.00	0.44
1:A:52:LEU:HD11	1:A:68:ILE:HA	2.00	0.44
1:A:227:HIS:HA	1:A:228:PRO:HD3	1.86	0.44
1:B:48:MET:HE2	1:B:48:MET:HA	1.99	0.44
1:B:197:LEU:CD2	1:B:395:VAL:HG12	2.47	0.44
1:D:170:HIS:HD2	1:D:211:GLU:HG2	1.80	0.44
1:A:67:THR:O	1:A:71:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ILE:HD11	1:C:74:LEU:HD22	1.99	0.44
1:B:488:ASP:OD1	1:B:490:LEU:HB2	2.18	0.43
1:D:266:MET:HE2	1:D:269:LEU:HD23	1.99	0.43
1:A:9:VAL:O	1:A:11:ILE:HG12	2.18	0.43
1:C:383:VAL:O	1:C:387:VAL:HG23	2.19	0.43
1:D:49:ASP:HB3	1:D:62:THR:O	2.18	0.43
1:D:480:ASP:HB3	1:D:485:LYS:O	2.18	0.43
1:A:326:LYS:HB3	1:A:370:LYS:HB2	1.99	0.43
1:B:416:ILE:HD13	1:B:466:VAL:HG12	2.00	0.43
1:B:506:LYS:O	1:B:510:GLU:HG3	2.19	0.43
1:D:108:LEU:CD2	1:D:516:LEU:HD13	2.48	0.43
1:A:163:THR:HG22	1:A:171:LYS:HZ2	1.78	0.43
1:B:334:THR:HG22	1:B:335:ASN:ND2	2.34	0.43
1:C:243:ASN:O	1:C:295:LYS:HG2	2.19	0.43
1:D:88:THR:HA	1:D:91:LYS:HZ2	1.83	0.43
1:D:501:LYS:HE3	1:D:501:LYS:HA	2.00	0.43
1:A:37:GLU:O	1:A:40:ARG:HG2	2.18	0.43
1:D:190:ASP:OD2	1:D:190:ASP:O	2.37	0.43
1:D:204:LYS:HD3	1:D:388:GLU:OE2	2.18	0.43
1:D:227:HIS:HB3	1:D:230:MET:HG3	2.01	0.43
1:A:266:MET:O	1:A:270:GLU:HG3	2.19	0.43
1:C:269:LEU:HD12	1:C:269:LEU:HA	1.92	0.43
1:B:370:LYS:HE3	4:B:2087:HOH:O	2.17	0.43
1:C:123:ILE:HG21	1:C:432:LYS:HB2	2.01	0.43
1:A:157:ILE:HD13	1:A:495:ILE:HG13	2.00	0.43
1:A:356:ALA:O	1:A:358:GLU:HG2	2.19	0.43
1:A:449:LYS:HG3	1:A:459:THR:OG1	2.18	0.43
1:C:413:ALA:HB3	1:C:414:PRO:HD3	1.99	0.43
1:D:450:THR:HG22	4:D:4013:HOH:O	2.18	0.43
1:A:103:ILE:HG12	1:A:446:ILE:HD11	2.00	0.42
1:B:121:PRO:O	1:B:125:THR:HB	2.19	0.42
1:B:170:HIS:HD2	1:B:211:GLU:HG2	1.78	0.42
1:C:49:ASP:OD1	1:C:63:ASN:HB2	2.18	0.42
1:D:334:THR:HG22	1:D:335:ASN:HD22	1.83	0.42
1:A:98:THR:O	1:A:102:VAL:HG23	2.19	0.42
1:C:106:GLU:CB	1:C:446:ILE:HG12	2.49	0.42
1:C:195:VAL:O	1:C:399:LYS:HE2	2.18	0.42
1:D:88:THR:HA	1:D:91:LYS:NZ	2.34	0.42
1:A:215:LEU:HD11	1:A:372:VAL:HG13	2.00	0.42
1:B:445:LYS:C	1:B:448:PRO:HD2	2.44	0.42
1:A:230:MET:HE1	1:A:312:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LYS:C	1:A:355:LEU:HD12	2.44	0.42
1:D:244:GLU:CB	1:D:334:THR:O	2.66	0.42
1:B:259:ILE:CD1	1:B:265:LEU:HD23	2.49	0.42
1:B:303:HIS:HD2	4:B:2090:HOH:O	2.02	0.42
1:C:184:GLN:NE2	1:C:184:GLN:HA	2.34	0.42
1:D:190:ASP:O	1:D:192:LYS:N	2.52	0.42
1:A:33:ARG:O	1:A:37:GLU:HG3	2.19	0.42
1:A:257:ILE:C	1:A:258:ASN:HD22	2.27	0.42
1:C:235:GLU:OE2	1:C:235:GLU:HA	2.20	0.42
1:D:282:HIS:HE1	1:D:339:LEU:O	2.01	0.42
1:A:257:ILE:HB	1:B:255:ALA:CB	2.49	0.42
1:B:313:VAL:HG21	1:B:361:ILE:HD13	2.02	0.42
1:D:52:LEU:HD11	1:D:68:ILE:HA	2.02	0.42
1:D:197:LEU:HD22	1:D:395:VAL:HG13	1.99	0.42
1:A:51:MET:HE2	1:B:521:VAL:HG13	2.02	0.42
1:A:205:LYS:HA	1:A:205:LYS:HD3	1.83	0.42
1:C:514:MET:HE3	1:D:166:ASN:HD21	1.84	0.42
1:D:165:LYS:C	1:D:166:ASN:O	2.59	0.42
1:D:217:ARG:HA	1:D:372:VAL:HG22	2.02	0.42
1:A:76:HIS:HD2	1:A:78:ALA:H	1.66	0.42
1:B:35:ILE:HD13	1:B:35:ILE:HA	1.89	0.42
1:B:146:VAL:HG22	1:B:147:ASP:H	1.85	0.42
1:C:98:THR:O	1:C:102:VAL:HG23	2.20	0.42
1:A:62:THR:CG2	1:A:386:GLU:OE2	2.68	0.42
1:A:166:ASN:CB	1:B:517:ARG:HD2	2.35	0.42
1:A:227:HIS:HD2	1:A:229:ARG:HB2	1.84	0.41
1:B:230:MET:HE1	1:B:312:ALA:HB3	2.02	0.41
1:B:378:GLY:N	1:B:384:ILE:HD11	2.35	0.41
1:B:470:HIS:HA	1:B:477:ILE:HB	2.02	0.41
1:A:110:LYS:HD2	1:A:442:ASP:OD1	2.20	0.41
1:B:195:VAL:HB	1:B:399:LYS:HG3	2.02	0.41
1:C:76:HIS:HA	1:C:77:PRO:HD3	1.93	0.41
1:C:165:LYS:HE2	4:C:3120:HOH:O	2.18	0.41
1:A:330:ALA:HB2	1:A:345:GLY:CA	2.51	0.41
1:B:276:LEU:HD13	1:B:300:LEU:HB3	2.03	0.41
1:A:490:LEU:HD12	1:A:490:LEU:HA	1.93	0.41
1:C:76:HIS:CD2	1:C:77:PRO:HD2	2.55	0.41
1:C:276:LEU:HD12	1:C:276:LEU:HA	1.95	0.41
1:C:372:VAL:HG13	1:C:373:THR:N	2.35	0.41
1:A:49:ASP:OD1	1:A:63:ASN:HB2	2.21	0.41
1:B:190:ASP:C	1:B:192:LYS:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:HB	1:B:255:ALA:HB2	2.01	0.41
1:A:399:LYS:HZ2	1:A:403:GLU:CD	2.29	0.41
1:B:218:GLY:HA3	1:B:363:VAL:O	2.21	0.41
1:B:283:ILE:HG21	1:B:291:VAL:HG21	2.02	0.41
1:B:352:GLU:HA	1:B:360:MET:O	2.20	0.41
1:B:516:LEU:HD12	1:B:516:LEU:HA	1.88	0.41
1:C:165:LYS:O	1:C:168:GLU:HG2	2.20	0.41
1:C:215:LEU:HD11	1:C:372:VAL:HG11	2.01	0.41
1:D:148:PRO:O	1:D:402:MET:HG2	2.21	0.41
1:D:397:VAL:HB	1:D:497:PRO:HG2	2.03	0.41
1:D:459:THR:HG22	1:D:460:VAL:N	2.35	0.41
1:A:240:ALA:HB3	1:A:291:VAL:HG22	2.03	0.41
1:A:415:GLU:CD	1:A:415:GLU:H	2.28	0.41
1:C:151:GLU:HG2	1:C:155:LEU:HD22	2.02	0.41
1:B:67:THR:O	1:B:71:LYS:HG2	2.20	0.41
1:C:29:ILE:HD13	1:C:112:GLU:HB2	2.02	0.41
1:C:163:THR:HG22	1:C:171:LYS:NZ	2.36	0.41
1:D:171:LYS:HG3	1:D:172:GLU:N	2.36	0.41
1:A:146:VAL:CG2	1:A:147:ASP:N	2.84	0.41
1:A:470:HIS:HA	1:A:477:ILE:HB	2.03	0.41
1:B:217:ARG:HA	1:B:372:VAL:HG23	2.03	0.41
1:C:127:GLY:HA3	1:C:436:ALA:HB3	2.03	0.41
1:D:204:LYS:HB3	1:D:384:ILE:HG23	2.03	0.41
1:A:18:ARG:HA	1:A:521:VAL:O	2.20	0.40
1:B:239:ILE:HD11	1:B:347:ALA:HB2	2.03	0.40
1:B:396:LYS:HG3	4:B:2083:HOH:O	2.19	0.40
1:C:146:VAL:CG2	1:C:153:THR:HG21	2.37	0.40
1:D:76:HIS:CD2	1:D:78:ALA:HB3	2.56	0.40
1:D:384:ILE:HG22	1:D:385:ASP:N	2.36	0.40
1:A:106:GLU:HB2	1:A:446:ILE:HG12	2.03	0.40
1:A:404:ASP:O	1:A:406:ALA:N	2.50	0.40
1:A:473:ARG:HB2	1:A:477:ILE:HG13	2.03	0.40
1:A:154:LEU:HG	1:A:398:VAL:HG13	2.04	0.40
1:A:446:ILE:HD12	1:A:447:ILE:N	2.37	0.40
1:A:463:LEU:HD13	1:A:463:LEU:HA	1.90	0.40
1:A:480:ASP:OD2	1:A:480:ASP:C	2.64	0.40
1:B:110:LYS:HA	1:B:110:LYS:HE2	2.02	0.40
1:B:203:GLU:CG	1:B:360:MET:HE1	2.51	0.40
1:C:296:GLY:HA2	1:C:315:ARG:HD2	2.02	0.40
1:D:227:HIS:HA	1:D:228:PRO:HD3	1.86	0.40
1:D:367:LYS:HB3	1:D:367:LYS:NZ	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:ILE:O	1:D:450:THR:CG2	2.53	0.40
1:D:458:ASP:OD2	1:D:458:ASP:C	2.62	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1162:HOH:O	4:B:2002:HOH:O[4_555]	0.56	1.64
4:C:3159:HOH:O	4:D:4143:HOH:O[4_555]	0.71	1.49
4:C:3137:HOH:O	4:D:4115:HOH:O[4_555]	0.74	1.46
1:C:272:GLU:OE2	1:D:253:THR:OG1[4_555]	2.01	0.19
4:C:3148:HOH:O	4:D:4139:HOH:O[4_555]	2.04	0.16
1:C:380:THR:OG1	1:D:84:GLU:OE1[4_555]	2.14	0.06
4:B:2067:HOH:O	4:D:4112:HOH:O[2_656]	2.15	0.05

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	516/548 (94%)	504 (98%)	10 (2%)	2 (0%)	30	38
1	B	516/548 (94%)	503 (98%)	10 (2%)	3 (1%)	21	27
1	C	516/548 (94%)	500 (97%)	12 (2%)	4 (1%)	16	20
1	D	516/548 (94%)	502 (97%)	11 (2%)	3 (1%)	21	27
All	All	2064/2192 (94%)	2009 (97%)	43 (2%)	12 (1%)	21	27

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	GLU
1	B	10	VAL

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Mol	Chain	Res	Type
1	B	235	GLU
1	C	235	GLU
1	D	235	GLU
1	D	367	LYS
1	A	367	LYS
1	B	367	LYS
1	C	190	ASP
1	C	367	LYS
1	D	190	ASP
1	C	10	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/441 (96%)	396 (94%)	27 (6%)	16	23
1	B	423/441 (96%)	398 (94%)	25 (6%)	18	26
1	C	423/441 (96%)	397 (94%)	26 (6%)	17	24
1	D	423/441 (96%)	389 (92%)	34 (8%)	11	15
All	All	1692/1764 (96%)	1580 (93%)	112 (7%)	15	21

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	62	THR
1	A	82	MET
1	A	107	LEU
1	A	154	LEU
1	A	155	LEU
1	A	171	LYS
1	A	238	LYS
1	A	241	LEU
1	A	246	LEU
1	A	258	ASN

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Mol	Chain	Res	Type
1	A	269	LEU
1	A	305	LEU
1	A	358	GLU
1	A	372	VAL
1	A	375	LEU
1	A	395	VAL
1	A	404	ASP
1	A	415	GLU
1	A	446	ILE
1	A	459	THR
1	A	463	LEU
1	A	490	LEU
1	A	496	GLU
1	A	498	LEU
1	A	501	LYS
1	A	516	LEU
1	B	14	GLU
1	B	30	LEU
1	B	82	MET
1	B	107	LEU
1	B	125	THR
1	B	147	ASP
1	B	154	LEU
1	B	155	LEU
1	B	169	SER
1	B	229	ARG
1	B	241	LEU
1	B	269	LEU
1	B	305	LEU
1	B	375	LEU
1	B	380	THR
1	B	415	GLU
1	B	423	ASP
1	B	435	LEU
1	B	446	ILE
1	B	463	LEU
1	B	483	GLU
1	B	490	LEU
1	B	498	LEU
1	B	501	LYS
1	B	516	LEU
1	C	14	GLU

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Mol	Chain	Res	Type
1	C	30	LEU
1	C	35	ILE
1	C	82	MET
1	C	107	LEU
1	C	125	THR
1	C	153	THR
1	C	154	LEU
1	C	155	LEU
1	C	241	LEU
1	C	246	LEU
1	C	269	LEU
1	C	305	LEU
1	C	372	VAL
1	C	375	LEU
1	C	415	GLU
1	C	435	LEU
1	C	446	ILE
1	C	450	THR
1	C	459	THR
1	C	463	LEU
1	C	483	GLU
1	C	490	LEU
1	C	498	LEU
1	C	501	LYS
1	C	516	LEU
1	D	14	GLU
1	D	17	GLN
1	D	30	LEU
1	D	58	ASP
1	D	82	MET
1	D	107	LEU
1	D	125	THR
1	D	152	GLU
1	D	154	LEU
1	D	155	LEU
1	D	163	THR
1	D	169	SER
1	D	211	GLU
1	D	229	ARG
1	D	241	LEU
1	D	246	LEU
1	D	269	LEU

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Mol	Chain	Res	Type
1	D	305	LEU
1	D	367	LYS
1	D	372	VAL
1	D	375	LEU
1	D	380	THR
1	D	384	ILE
1	D	395	VAL
1	D	404	ASP
1	D	415	GLU
1	D	435	LEU
1	D	446	ILE
1	D	450	THR
1	D	459	THR
1	D	490	LEU
1	D	498	LEU
1	D	501	LYS
1	D	516	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	75	GLN
1	A	76	HIS
1	A	89	GLN
1	A	117	GLN
1	A	118	ASN
1	A	184	GLN
1	A	227	HIS
1	A	258	ASN
1	A	282	HIS
1	A	285	GLN
1	A	368	ASN
1	B	28	ASN
1	B	76	HIS
1	B	89	GLN
1	B	118	ASN
1	B	170	HIS
1	B	184	GLN
1	B	282	HIS
1	B	285	GLN
1	B	303	HIS

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Mol	Chain	Res	Type
1	B	368	ASN
1	B	503	GLN
1	C	28	ASN
1	C	76	HIS
1	C	89	GLN
1	C	117	GLN
1	C	118	ASN
1	C	170	HIS
1	C	184	GLN
1	C	199	ASN
1	C	227	HIS
1	C	282	HIS
1	C	285	GLN
1	C	294	GLN
1	C	303	HIS
1	C	335	ASN
1	C	368	ASN
1	C	382	HIS
1	C	428	GLN
1	C	503	GLN
1	D	17	GLN
1	D	28	ASN
1	D	75	GLN
1	D	76	HIS
1	D	89	GLN
1	D	118	ASN
1	D	170	HIS
1	D	184	GLN
1	D	199	ASN
1	D	227	HIS
1	D	282	HIS
1	D	285	GLN
1	D	294	GLN
1	D	303	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	ANP	C	3528	2	33,33,33	1.55	7 (21%)	45,52,52	1.21	3 (6%)
3	ANP	A	1528	2	33,33,33	1.56	7 (21%)	45,52,52	1.18	2 (4%)
3	ANP	B	2528	2	33,33,33	1.49	7 (21%)	45,52,52	1.25	2 (4%)
3	ANP	D	4528	2	33,33,33	1.51	7 (21%)	45,52,52	1.23	2 (4%)

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
3	ANP	C	3528	2	-	4/18/38/38	0/3/3/3
3	ANP	A	1528	2	-	4/18/38/38	0/3/3/3
3	ANP	B	2528	2	-	4/18/38/38	0/3/3/3
3	ANP	D	4528	2	-	4/18/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3528	ANP	PA-O3A	3.73	1.63	1.59
3	A	1528	ANP	PB-O3A	3.70	1.63	1.59
3	A	1528	ANP	PA-O3A	3.51	1.63	1.59
3	D	4528	ANP	PB-O3A	3.46	1.63	1.59
3	A	1528	ANP	PB-O2B	-3.42	1.47	1.56
3	D	4528	ANP	PB-O2B	-3.39	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2528	ANP	PB-O2B	-3.37	1.47	1.56
3	C	3528	ANP	PB-O2B	-3.36	1.47	1.56
3	B	2528	ANP	PA-O3A	3.31	1.63	1.59
3	D	4528	ANP	PA-O3A	3.29	1.63	1.59
3	B	2528	ANP	PB-O3A	3.02	1.62	1.59
3	C	3528	ANP	PG-O2G	-3.01	1.48	1.56
3	C	3528	ANP	PB-O3A	2.97	1.62	1.59
3	D	4528	ANP	PG-O2G	-2.94	1.49	1.56
3	B	2528	ANP	PG-O2G	-2.89	1.49	1.56
3	A	1528	ANP	PG-O2G	-2.84	1.49	1.56
3	A	1528	ANP	PG-O3G	-2.78	1.49	1.56
3	C	3528	ANP	PG-O3G	-2.73	1.49	1.56
3	B	2528	ANP	PG-O3G	-2.51	1.50	1.56
3	D	4528	ANP	PG-O3G	-2.46	1.50	1.56
3	C	3528	ANP	PG-O1G	2.41	1.49	1.46
3	D	4528	ANP	C4-N3	2.33	1.38	1.34
3	A	1528	ANP	C4-N3	2.31	1.38	1.34
3	C	3528	ANP	C4-N3	2.28	1.38	1.34
3	B	2528	ANP	C4-N3	2.27	1.38	1.34
3	A	1528	ANP	PG-O1G	2.22	1.49	1.46
3	B	2528	ANP	PG-O1G	2.20	1.49	1.46
3	D	4528	ANP	PG-O1G	2.10	1.49	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1528	ANP	O2B-PB-O1B	4.59	119.71	109.87
3	B	2528	ANP	O2B-PB-O1B	4.49	119.50	109.87
3	D	4528	ANP	O2B-PB-O1B	4.43	119.37	109.87
3	C	3528	ANP	O2B-PB-O1B	4.21	118.90	109.87
3	B	2528	ANP	O1G-PG-N3B	3.01	116.20	111.77
3	D	4528	ANP	O1G-PG-N3B	-2.85	107.58	111.77
3	C	3528	ANP	O1G-PG-N3B	-2.64	107.88	111.77
3	A	1528	ANP	O1B-PB-N3B	-2.21	108.51	111.77
3	C	3528	ANP	O1B-PB-N3B	-2.05	108.75	111.77

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1528	ANP	PB-N3B-PG-O1G
3	A	1528	ANP	PG-N3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	A	1528	ANP	PA-O3A-PB-O2B
3	B	2528	ANP	PB-N3B-PG-O1G
3	B	2528	ANP	PG-N3B-PB-O1B
3	B	2528	ANP	PA-O3A-PB-O2B
3	C	3528	ANP	PB-N3B-PG-O1G
3	C	3528	ANP	PG-N3B-PB-O1B
3	C	3528	ANP	PA-O3A-PB-O2B
3	D	4528	ANP	PB-N3B-PG-O1G
3	D	4528	ANP	PG-N3B-PB-O1B
3	D	4528	ANP	PA-O3A-PB-O2B
3	A	1528	ANP	PA-O3A-PB-O1B
3	B	2528	ANP	PA-O3A-PB-O1B
3	C	3528	ANP	PA-O3A-PB-O1B
3	D	4528	ANP	PA-O3A-PB-O1B

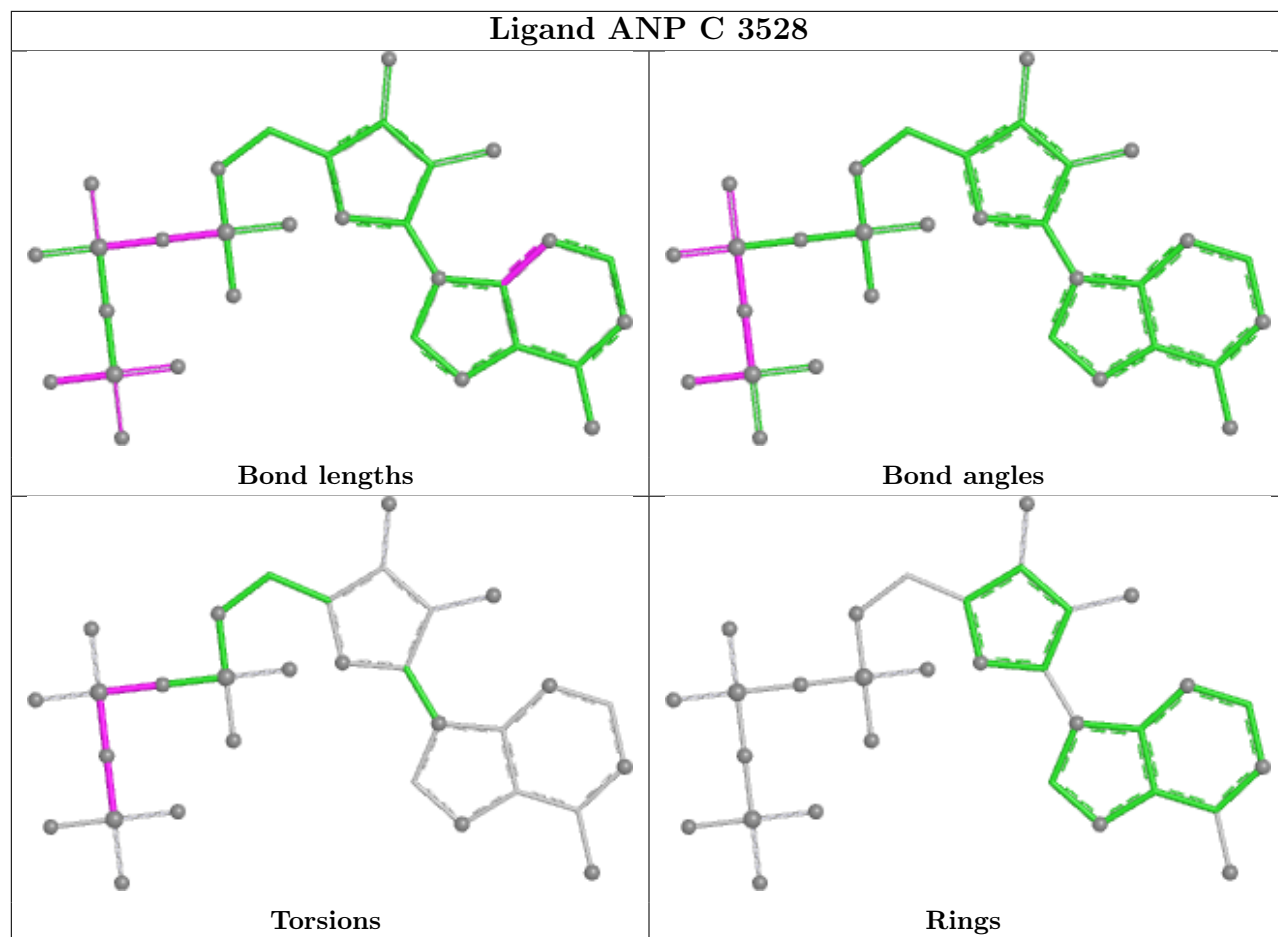
There are no ring outliers.

4 monomers are involved in 8 short contacts:

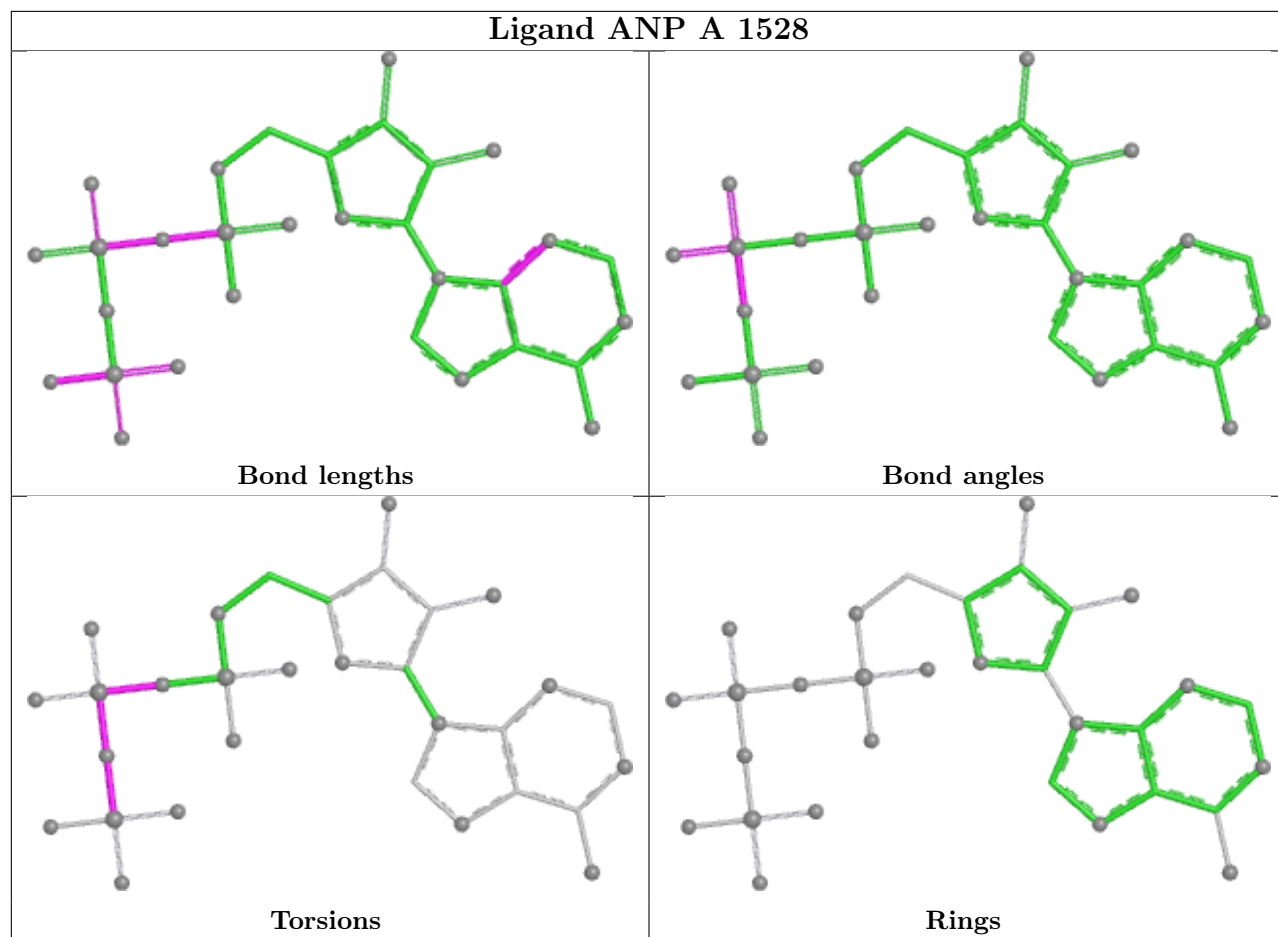
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3528	ANP	2	0
3	A	1528	ANP	2	0
3	B	2528	ANP	2	0
3	D	4528	ANP	2	0

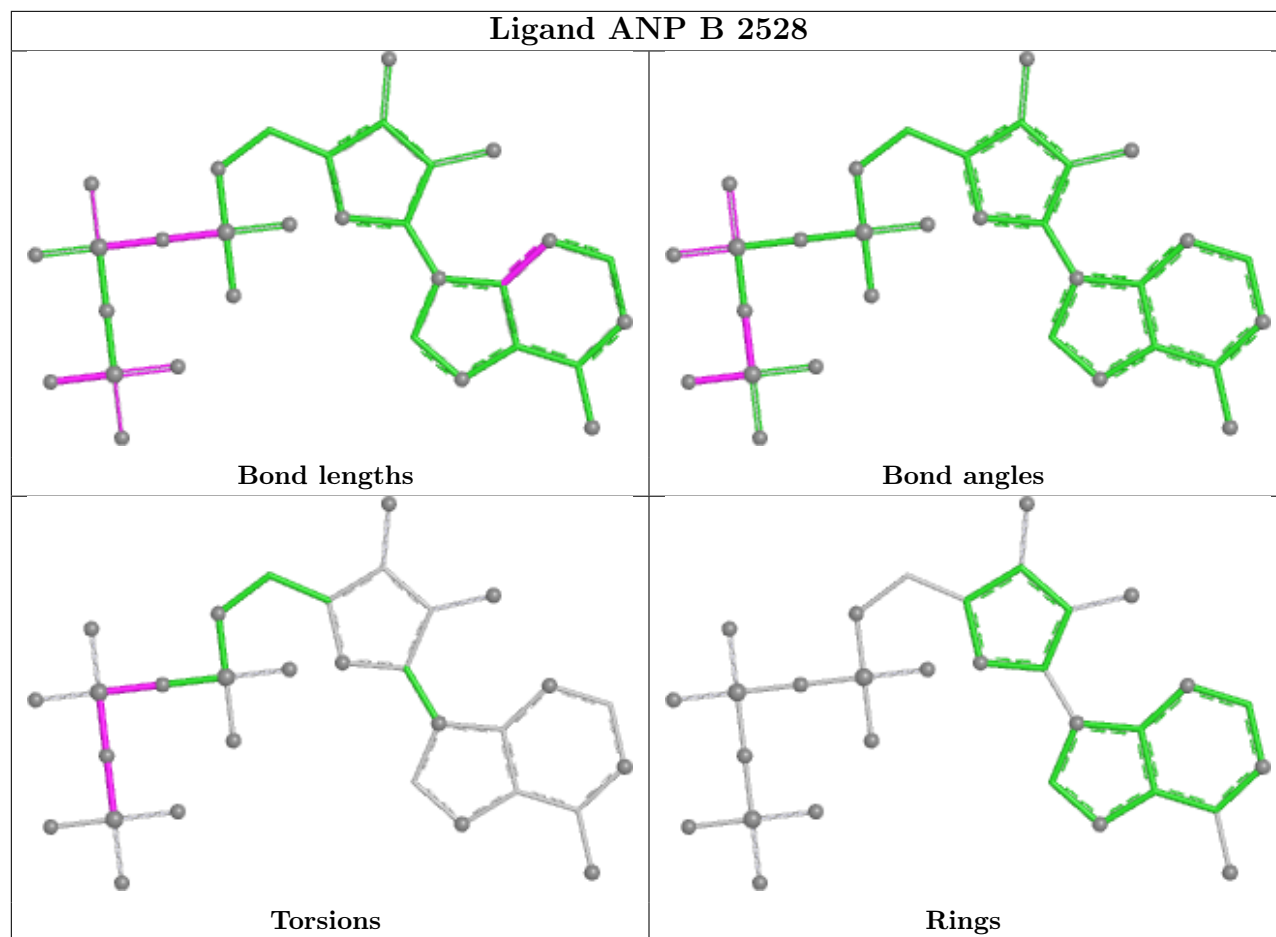
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

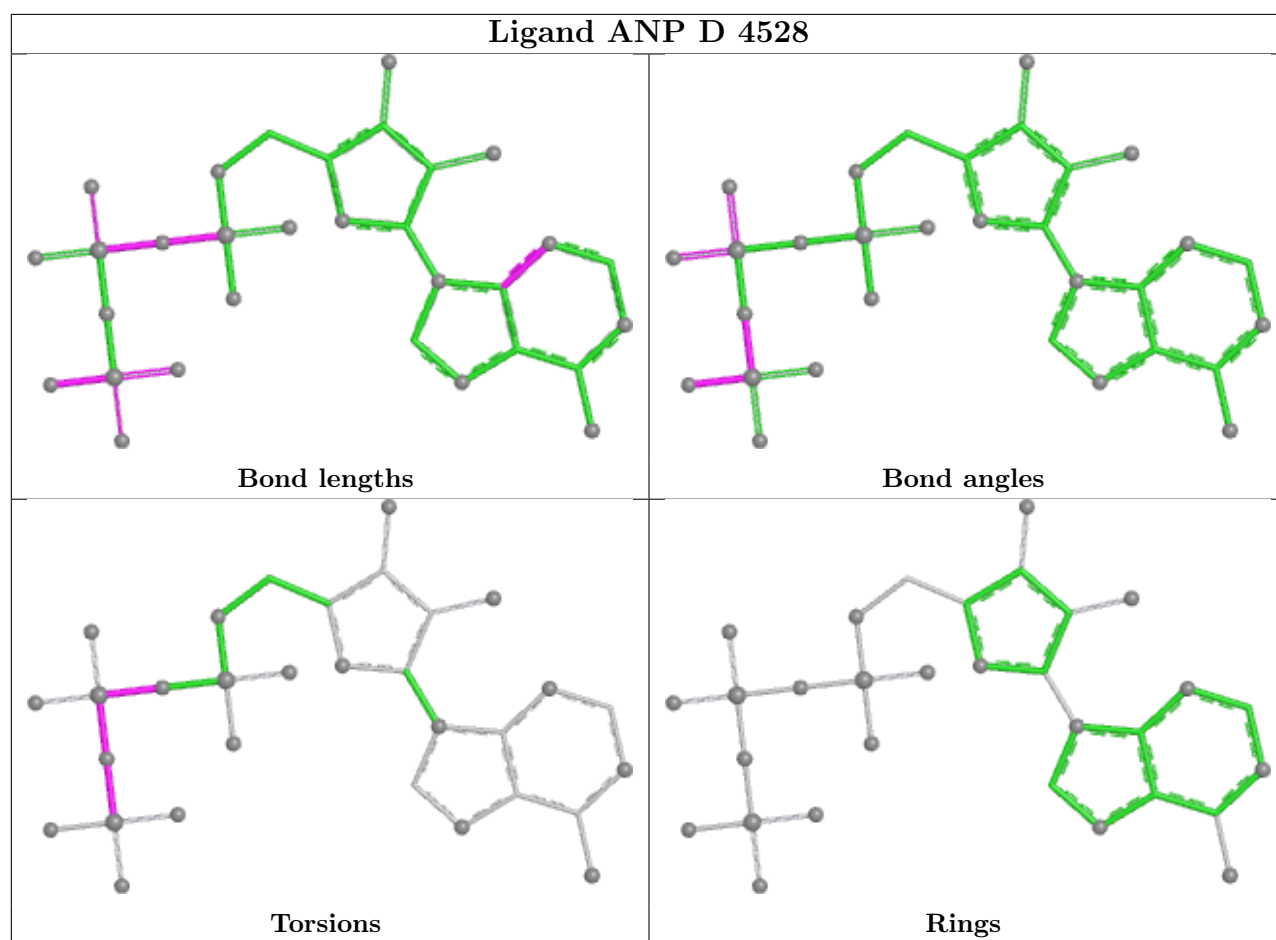
Ligand ANP C 3528



Ligand ANP A 1528







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	518/548 (94%)	1.16	70 (13%) 7 8	9, 23, 41, 83	0
1	B	518/548 (94%)	1.35	107 (20%) 2 3	11, 24, 40, 82	0
1	C	518/548 (94%)	1.60	142 (27%) 1 1	8, 22, 41, 77	0
1	D	518/548 (94%)	1.20	84 (16%) 4 5	11, 24, 41, 77	0
All	All	2072/2192 (94%)	1.33	403 (19%) 3 3	8, 23, 41, 83	0

All (403) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	VAL	8.8
1	D	9	VAL	8.4
1	A	526	ALA	8.0
1	B	9	VAL	7.1
1	C	9	VAL	7.0
1	D	526	ALA	6.7
1	D	191	GLY	6.3
1	C	526	ALA	6.1
1	C	58	ASP	6.1
1	B	526	ALA	6.0
1	C	191	GLY	5.6
1	B	188	LYS	5.6
1	A	192	LYS	5.2
1	B	191	GLY	5.1
1	C	308	TYR	4.8
1	C	229	ARG	4.7
1	B	308	TYR	4.7
1	C	357	GLY	4.6
1	A	10	VAL	4.6
1	A	166	ASN	4.5
1	C	356	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	72	ILE	4.5
1	C	57	GLY	4.5
1	D	166	ASN	4.5
1	C	189	LYS	4.5
1	B	192	LYS	4.4
1	D	192	LYS	4.4
1	C	192	LYS	4.4
1	B	190	ASP	4.4
1	C	235	GLU	4.3
1	A	189	LYS	4.2
1	B	483	GLU	4.2
1	D	235	GLU	4.2
1	B	189	LYS	4.1
1	C	55	SER	4.1
1	A	525	LYS	4.1
1	A	190	ASP	4.0
1	C	355	LEU	4.0
1	C	193	TYR	4.0
1	C	72	ILE	4.0
1	D	525	LYS	3.9
1	D	11	ILE	3.9
1	C	10	VAL	3.9
1	A	258	ASN	3.9
1	D	10	VAL	3.8
1	D	72	ILE	3.8
1	B	304	TYR	3.8
1	C	164	GLY	3.8
1	C	269	LEU	3.8
1	C	287	GLY	3.8
1	B	367	LYS	3.7
1	C	265	LEU	3.7
1	B	10	VAL	3.7
1	C	349	VAL	3.7
1	D	55	SER	3.7
1	A	243	ASN	3.6
1	B	258	ASN	3.6
1	D	13	PRO	3.6
1	A	188	LYS	3.6
1	A	191	GLY	3.6
1	A	12	LEU	3.6
1	C	363	VAL	3.6
1	A	235	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	189	LYS	3.5
1	A	404	ASP	3.5
1	D	404	ASP	3.5
1	A	13	PRO	3.5
1	D	357	GLY	3.5
1	B	58	ASP	3.5
1	C	231	PRO	3.5
1	C	227	HIS	3.5
1	C	384	ILE	3.5
1	C	190	ASP	3.5
1	D	190	ASP	3.5
1	C	218	GLY	3.4
1	B	259	ILE	3.4
1	C	335	ASN	3.4
1	D	56	LEU	3.4
1	C	367	LYS	3.4
1	A	15	GLY	3.4
1	D	243	ASN	3.4
1	D	265	LEU	3.3
1	A	381	GLU	3.3
1	B	193	TYR	3.3
1	B	313	VAL	3.3
1	A	11	ILE	3.3
1	B	13	PRO	3.3
1	C	380	THR	3.3
1	B	266	MET	3.2
1	A	259	ILE	3.2
1	B	482	PHE	3.2
1	C	482	PHE	3.2
1	C	315	ARG	3.2
1	B	231	PRO	3.2
1	D	268	PHE	3.2
1	C	267	SER	3.2
1	C	225	VAL	3.2
1	D	258	ASN	3.2
1	C	56	LEU	3.2
1	B	247	GLU	3.2
1	C	243	ASN	3.2
1	D	17	GLN	3.2
1	C	353	ARG	3.1
1	C	188	LYS	3.1
1	A	187	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	235	GLU	3.1
1	B	336	VAL	3.1
1	B	11	ILE	3.1
1	D	337	LYS	3.1
1	B	433	GLU	3.1
1	C	220	VAL	3.1
1	C	304	TYR	3.1
1	C	346	TYR	3.1
1	C	259	ILE	3.1
1	C	405	GLY	3.1
1	C	226	VAL	3.1
1	D	367	LYS	3.1
1	B	357	GLY	3.1
1	C	258	ASN	3.1
1	D	188	LYS	3.1
1	B	265	LEU	3.1
1	B	261	SER	3.0
1	A	298	ASP	3.0
1	B	243	ASN	3.0
1	D	336	VAL	3.0
1	D	259	ILE	3.0
1	D	58	ASP	3.0
1	B	455	ALA	3.0
1	C	332	ILE	3.0
1	A	367	LYS	3.0
1	D	14	GLU	3.0
1	C	292	PHE	2.9
1	D	356	ALA	2.9
1	A	56	LEU	2.9
1	C	525	LYS	2.9
1	B	229	ARG	2.9
1	D	41	THR	2.9
1	A	461	GLU	2.9
1	C	329	GLY	2.9
1	D	275	MET	2.9
1	C	263	ASP	2.9
1	A	22	ARG	2.9
1	B	302	GLN	2.9
1	C	311	MET	2.9
1	B	55	SER	2.9
1	A	255	ALA	2.9
1	B	14	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	358	GLU	2.9
1	C	483	GLU	2.9
1	D	187	GLU	2.9
1	D	261	SER	2.8
1	D	229	ARG	2.8
1	D	12	LEU	2.8
1	C	54	ASP	2.8
1	C	228	PRO	2.8
1	A	17	GLN	2.8
1	D	304	TYR	2.8
1	C	291	VAL	2.8
1	B	298	ASP	2.8
1	C	261	SER	2.8
1	C	456	GLY	2.8
1	B	306	ALA	2.8
1	C	312	ALA	2.8
1	A	357	GLY	2.8
1	C	224	GLU	2.8
1	C	305	LEU	2.8
1	A	167	ALA	2.8
1	D	483	GLU	2.7
1	C	41	THR	2.7
1	C	163	THR	2.7
1	C	285	GLN	2.7
1	C	340	THR	2.7
1	D	302	GLN	2.7
1	C	237	ALA	2.7
1	C	347	ALA	2.7
1	B	260	THR	2.7
1	C	236	ASN	2.7
1	A	162	ILE	2.7
1	A	169	SER	2.7
1	A	358	GLU	2.7
1	A	27	LEU	2.7
1	A	304	TYR	2.7
1	C	302	GLN	2.7
1	B	225	VAL	2.7
1	B	335	ASN	2.7
1	D	381	GLU	2.7
1	D	57	GLY	2.7
1	C	233	ARG	2.7
1	B	53	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	287	GLY	2.6
1	C	242	ILE	2.6
1	C	493	GLY	2.6
1	B	311	MET	2.6
1	D	303	HIS	2.6
1	C	205	LYS	2.6
1	A	245	ALA	2.6
1	C	306	ALA	2.6
1	D	424	GLU	2.6
1	D	263	ASP	2.6
1	D	298	ASP	2.6
1	C	365	GLY	2.6
1	C	78	ALA	2.6
1	C	455	ALA	2.6
1	D	22	ARG	2.6
1	B	368	ASN	2.6
1	A	260	THR	2.6
1	B	372	VAL	2.6
1	C	381	GLU	2.6
1	B	349	VAL	2.6
1	B	187	GLU	2.5
1	D	355	LEU	2.5
1	B	288	ALA	2.5
1	B	356	ALA	2.5
1	D	299	ASP	2.5
1	B	292	PHE	2.5
1	C	362	PHE	2.5
1	C	354	LYS	2.5
1	B	428	GLN	2.5
1	C	266	MET	2.5
1	B	524	ALA	2.5
1	C	394	ALA	2.5
1	B	57	GLY	2.5
1	C	484	GLY	2.5
1	D	87	LYS	2.5
1	B	363	VAL	2.5
1	D	83	VAL	2.5
1	D	194	VAL	2.5
1	B	22	ARG	2.5
1	B	315	ARG	2.5
1	A	147	ASP	2.5
1	D	116	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	366	CYS	2.5
1	D	227	HIS	2.5
1	A	14	GLU	2.5
1	A	194	VAL	2.5
1	C	319	SER	2.5
1	D	308	TYR	2.5
1	D	266	MET	2.5
1	C	289	ASN	2.5
1	D	524	ALA	2.5
1	C	207	GLY	2.5
1	B	381	GLU	2.4
1	C	491	GLU	2.4
1	B	194	VAL	2.4
1	C	234	VAL	2.4
1	C	268	PHE	2.4
1	C	290	VAL	2.4
1	B	525	LYS	2.4
1	B	303	HIS	2.4
1	A	315	ARG	2.4
1	C	14	GLU	2.4
1	C	211	GLU	2.4
1	B	334	THR	2.4
1	B	380	THR	2.4
1	D	380	THR	2.4
1	C	59	ILE	2.4
1	C	283	ILE	2.4
1	C	313	VAL	2.4
1	B	236	ASN	2.4
1	D	315	ARG	2.4
1	B	167	ALA	2.4
1	D	167	ALA	2.4
1	B	494	ILE	2.4
1	C	372	VAL	2.4
1	B	276	LEU	2.4
1	C	300	LEU	2.4
1	D	19	TYR	2.4
1	A	186	ALA	2.4
1	B	279	MET	2.4
1	C	374	ILE	2.4
1	A	303	HIS	2.4
1	C	22	ARG	2.4
1	B	424	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	228	PRO	2.3
1	A	72	ILE	2.3
1	C	11	ILE	2.3
1	C	216	VAL	2.3
1	C	239	ILE	2.3
1	C	336	VAL	2.3
1	D	482	PHE	2.3
1	A	300	LEU	2.3
1	C	247	GLU	2.3
1	D	272	GLU	2.3
1	C	330	ALA	2.3
1	D	251	THR	2.3
1	C	217	ARG	2.3
1	A	522	ILE	2.3
1	C	162	ILE	2.3
1	D	446	ILE	2.3
1	C	358	GLU	2.3
1	D	350	VAL	2.3
1	A	335	ASN	2.3
1	C	171	LYS	2.3
1	B	405	GLY	2.3
1	A	163	THR	2.3
1	B	267	SER	2.3
1	D	285	GLN	2.3
1	C	368	ASN	2.3
1	D	368	ASN	2.3
1	C	47	GLY	2.3
1	C	240	ALA	2.3
1	B	234	VAL	2.3
1	C	53	VAL	2.3
1	C	276	LEU	2.2
1	D	472	ASN	2.2
1	B	493	GLY	2.2
1	C	275	MET	2.2
1	D	365	GLY	2.2
1	A	284	ALA	2.2
1	C	303	HIS	2.2
1	D	247	GLU	2.2
1	D	347	ALA	2.2
1	B	163	THR	2.2
1	C	17	GLN	2.2
1	A	277	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	150	ASP	2.2
1	A	405	GLY	2.2
1	B	94	GLY	2.2
1	C	378	GLY	2.2
1	D	287	GLY	2.2
1	D	288	ALA	2.2
1	D	312	ALA	2.2
1	A	308	TYR	2.2
1	D	267	SER	2.2
1	C	257	ILE	2.2
1	C	494	ILE	2.2
1	B	12	LEU	2.2
1	B	241	LEU	2.2
1	C	344	LEU	2.2
1	A	146	VAL	2.2
1	C	383	VAL	2.2
1	A	70	ASP	2.2
1	C	198	ASP	2.2
1	D	360	MET	2.2
1	A	282	HIS	2.2
1	C	167	ALA	2.2
1	B	283	ILE	2.2
1	D	257	ILE	2.2
1	B	353	ARG	2.2
1	A	58	ASP	2.2
1	A	519	ASP	2.2
1	B	224	GLU	2.2
1	C	277	LYS	2.2
1	D	491	GLU	2.2
1	A	524	ALA	2.2
1	B	169	SER	2.2
1	B	255	ALA	2.2
1	B	284	ALA	2.2
1	C	288	ALA	2.2
1	A	123	ILE	2.1
1	B	257	ILE	2.1
1	B	269	LEU	2.1
1	B	370	LYS	2.1
1	B	369	PRO	2.1
1	C	369	PRO	2.1
1	D	224	GLU	2.1
1	B	227	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	264	GLN	2.1
1	B	218	GLY	2.1
1	B	100	ALA	2.1
1	B	275	MET	2.1
1	B	355	LEU	2.1
1	A	254	ASP	2.1
1	B	54	ASP	2.1
1	B	180	GLU	2.1
1	B	254	ASP	2.1
1	B	491	GLU	2.1
1	D	76	HIS	2.1
1	C	487	ALA	2.1
1	C	524	ALA	2.1
1	A	271	GLN	2.1
1	B	285	GLN	2.1
1	B	164	GLY	2.1
1	A	261	SER	2.1
1	C	230	MET	2.1
1	B	272	GLU	2.1
1	B	27	LEU	2.1
1	B	332	ILE	2.1
1	C	280	VAL	2.1
1	C	398	VAL	2.1
1	B	337	LYS	2.0
1	B	286	THR	2.0
1	B	340	THR	2.0
1	D	358	GLU	2.0
1	C	282	HIS	2.0
1	A	119	ILE	2.0
1	B	239	ILE	2.0
1	C	262	PRO	2.0
1	B	293	VAL	2.0
1	A	307	LYS	2.0
1	C	337	LYS	2.0
1	A	244	GLU	2.0
1	C	352	GLU	2.0
1	C	360	MET	2.0
1	A	267	SER	2.0
1	A	450	THR	2.0
1	C	364	GLU	2.0
1	A	93	ALA	2.0
1	A	132	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	206	ALA	2.0
1	D	75	GLN	2.0
1	C	74	LEU	2.0
1	C	339	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

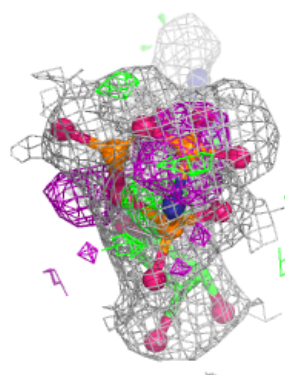
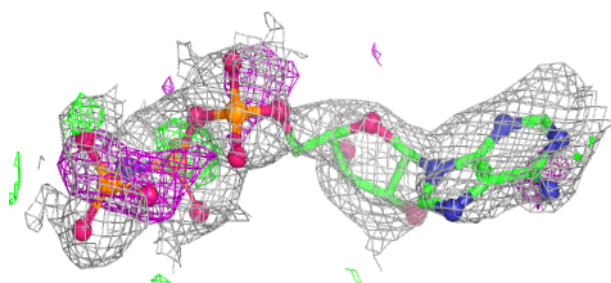
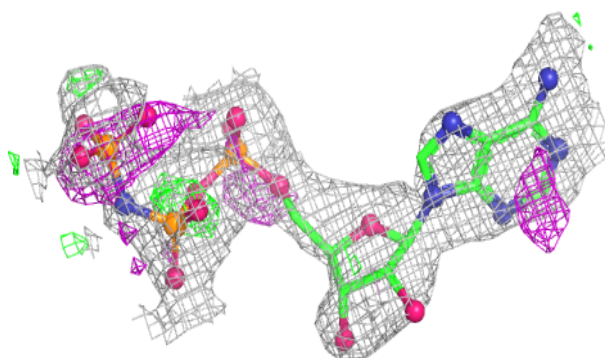
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	C	3527	1/1	0.48	0.39	85,85,85,85	0
2	MG	A	1527	1/1	0.68	0.35	71,71,71,71	0
2	MG	B	2527	1/1	0.71	0.26	39,39,39,39	0
3	ANP	C	3528	31/31	0.80	0.21	46,58,60,62	0
3	ANP	B	2528	31/31	0.83	0.19	50,59,65,66	0
2	MG	D	4527	1/1	0.84	0.21	57,57,57,57	0
3	ANP	A	1528	31/31	0.84	0.17	43,47,56,58	0
3	ANP	D	4528	31/31	0.84	0.19	46,54,57,60	0

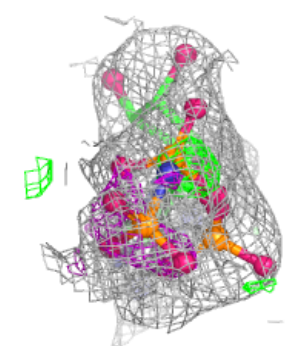
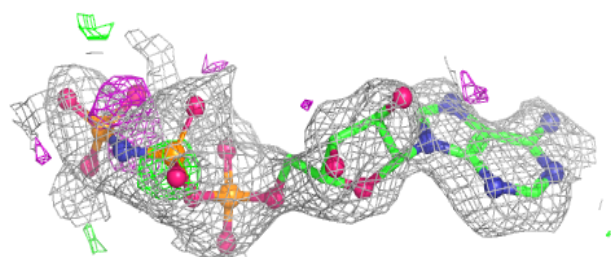
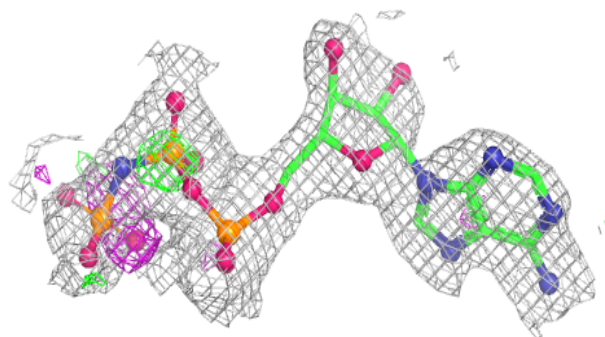
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP C 3528:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

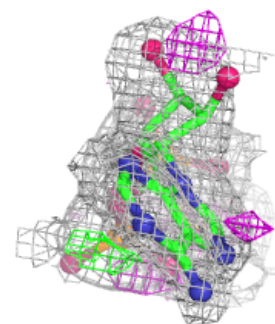
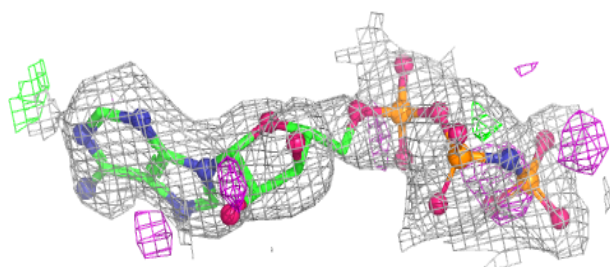
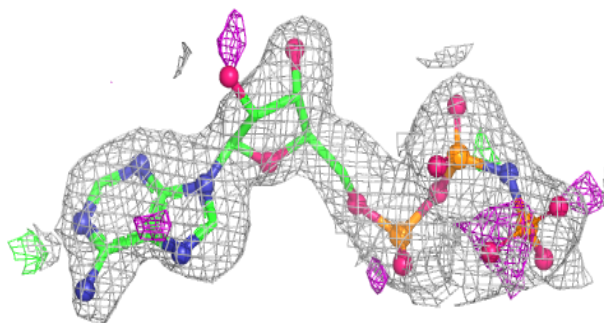
**Electron density around ANP B 2528:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

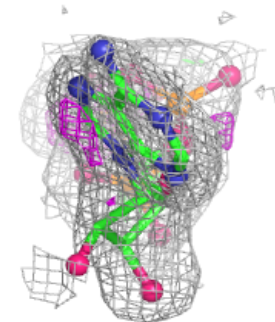
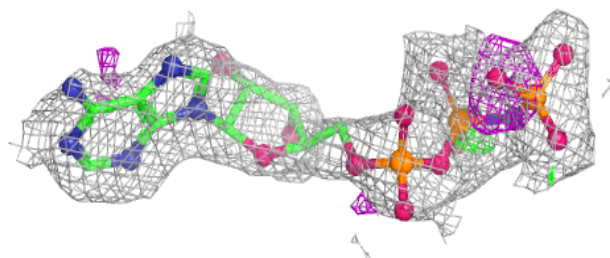
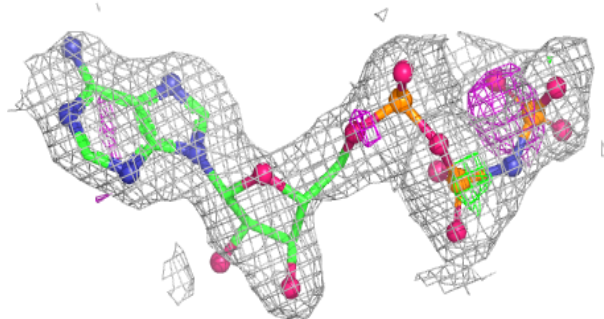


Electron density around ANP A 1528:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ANP D 4528:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.