



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 01:59 AM EDT

PDB ID : 1Q3Q
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

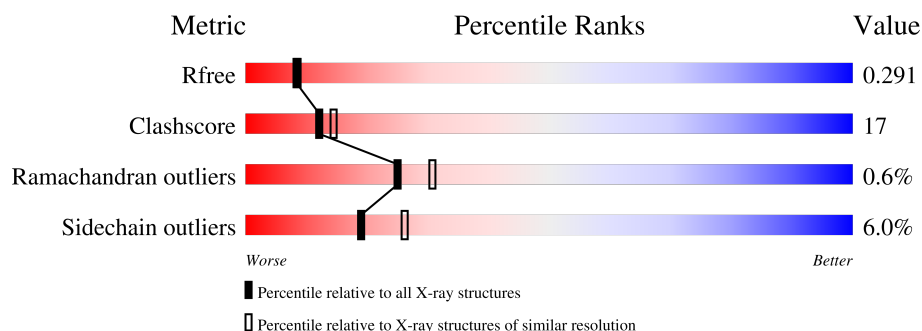
1 Overall quality at a glance

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	548	64% 28% • 5%
1	B	548	62% 30% • 5%
1	C	548	64% 27% • 5%
1	D	548	65% 25% • 5%

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			

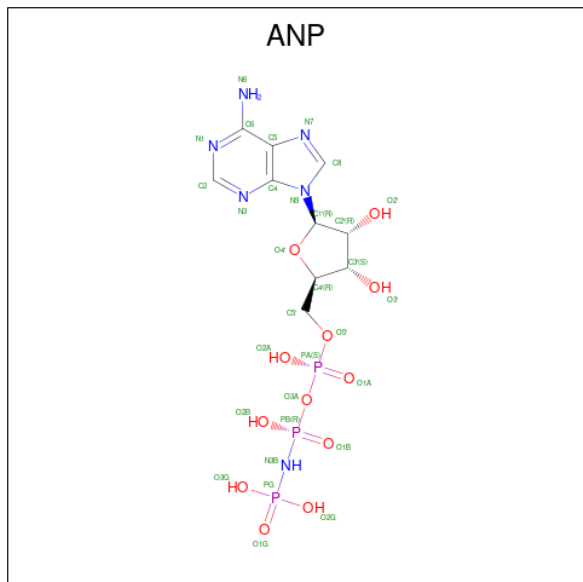
There are 8 discrepancies between the modelled and reference sequences:

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 (three-letter code: 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 (three-letter code: 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.

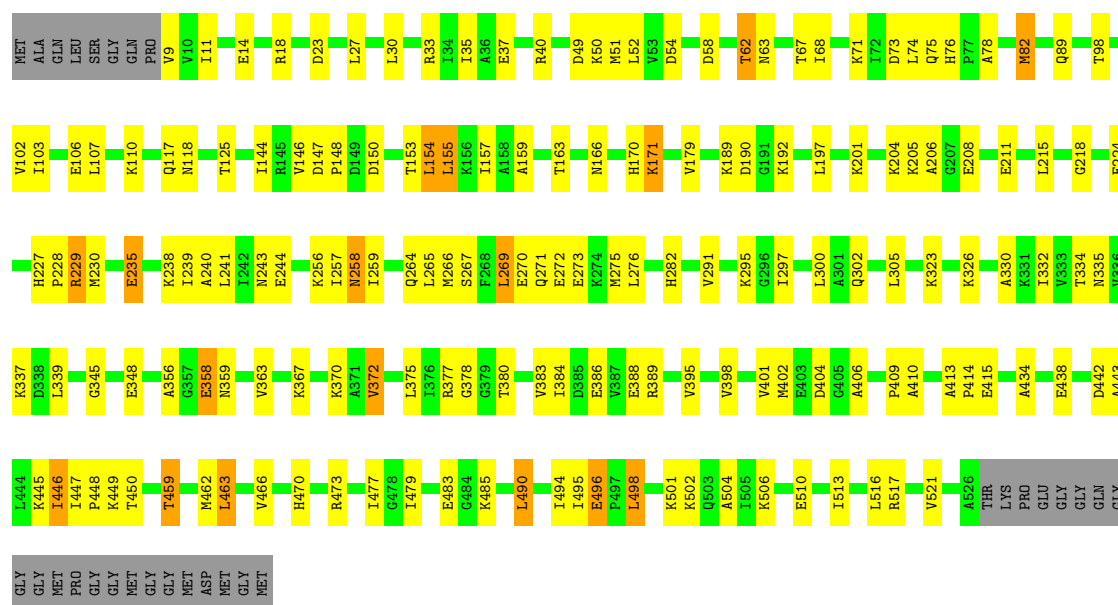
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total	O	0	0
			162	162		
4	B	174	Total	O	0	0
			174	174		
4	C	194	Total	O	0	0
			194	194		
4	D	164	Total	O	0	0
			164	164		

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. 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. 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.

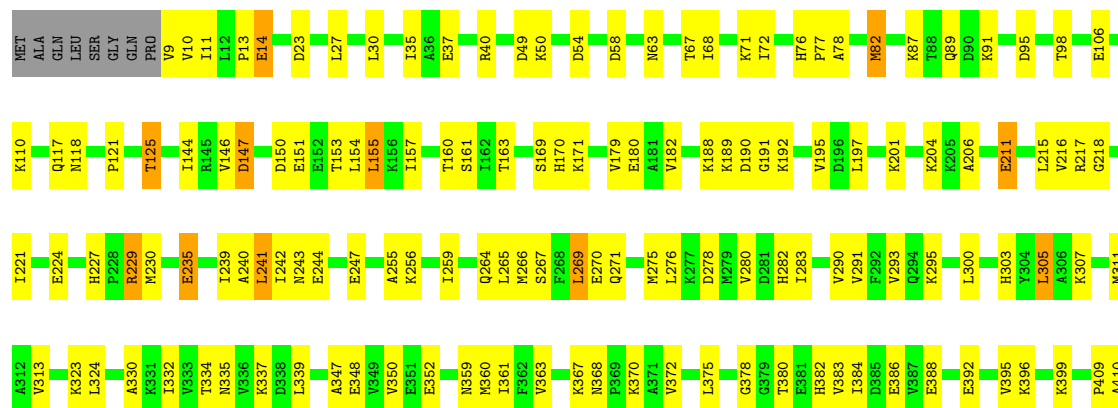
• Molecule 1: Thermosome alpha subunit

Chain A: 



• Molecule 1: Thermosome alpha subunit

Chain B: 





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 42.17 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.1 (41.97-2.30) 95.4 (42.17-2.30)	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 0.269 , 0.291	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 , 49.3	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/3982	0.61	0/5367
1	B	0.32	0/3982	0.60	0/5367
1	C	0.33	0/3982	0.61	0/5367
1	D	0.32	0/3982	0.61	0/5367
All	All	0.32	0/15928	0.61	0/21468

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3947	0	4127	148	0
1	B	3947	0	4127	145	0
1	C	3947	0	4127	148	2
1	D	3947	0	4127	144	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	554	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 17.

All (554) 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: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: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: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
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: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: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:163:THR:HG22	1:A:171:LYS:HZ2	1.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:466:VAL:HG21	1:A:479:ILE:HG12	1.66	0.75
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
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: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: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: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:A:189:LYS:HG2	1:A:192:LYS:O	1.93	0.69
1:B:163:THR:HB	1:B:171:LYS:HZ3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:380:THR:HG22	1:C:383:VAL:HG23	1.76	0.67
1:B:50:LYS:HD2	1:B:68:ILE:HD13	1.77	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: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:CE	1:A:82:MET:HA	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:LEU:HB3	1:B:332:ILE:HD13	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
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: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:D:190:ASP:C	1:D:192:LYS:H	2.00	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:266:MET:HE2	1:D:269:LEU:HD23	1.82	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: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: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:163:THR:HG22	1:A:171:LYS:HZ1	1.66	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:62:THR:HG22	1:C:63:ASN:H	1.67	0.59
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: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:191:GLY:C	1:C:192:LYS:HD2	2.25	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:B:433:GLU:H	1:B:433:GLU:CD	2.09	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: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:B:189:LYS:HG3	1:B:190:ASP:OD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:37:GLU:HA	1:B:40:ARG:HG2	1.90	0.54
1:D:445:LYS:C	1:D:448:PRO:HD2	2.27	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: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: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: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:91:LYS:HB2	1:D:91:LYS:HZ2	1.74	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:82:MET:CE	1:D:82:MET:HA	2.39	0.52
1:D:496:GLU:HG3	4:D:4061:HOH:O	2.09	0.52
1:A:82:MET:HA	1:A:82:MET:HE2	1.90	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:C:146:VAL:HG22	1:C:147:ASP:N	2.24	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: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: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:242:ILE:O	1:D:293:VAL:HA	2.11	0.51
1:B:82:MET:HA	1:B:82:MET:CE	2.41	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:D:272:GLU:HA	1:D:275:MET:CE	2.41	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
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:D:334:THR:HG22	1:D:335:ASN:ND2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:HD13	1:B:495:ILE:HG13	1.92	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: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:77:PRO:HB2	1:D:51:MET:HE1	1.94	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:B:190:ASP:C	1:B:192:LYS:H	2.16	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:D:415:GLU:H	1:D:415:GLU:CD	2.16	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: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:A:272:GLU:HA	1:A:275:MET:HE3	1.95	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:180:GLU:CD	1:D:215:LEU:HD23	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:9:VAL:HG13	1:C:9:VAL:O	2.14	0.48
1:C:76:HIS:HD2	1:C:78:ALA:H	1.60	0.48
1:A:272:GLU:HA	1:A:275:MET:CE	2.44	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:A:62:THR:HG23	1:A:389:ARG:NE	2.28	0.48
1:C:32:ALA:HB1	1:C:82:MET:HE2	1.95	0.48
1:D:266:MET:CE	1:D:269:LEU:HD23	2.42	0.48
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: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:192:LYS:HD2	1:C:192:LYS:N	2.29	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: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:271:GLN:HG3	1:B:275:MET:CE	2.45	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:190:ASP:C	1:C:192:LYS:H	2.18	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:190:ASP:C	1:D:192:LYS:N	2.68	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:D:353:ARG:HH22	1:D:364:GLU:CD	2.17	0.46
1:A:89:GLN:HE22	1:A:504:ALA:N	2.13	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: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:C:266:MET:HE2	1:C:269:LEU:HD23	1.98	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:D:227:HIS:CD2	1:D:229:ARG:H	2.33	0.46
1:D:272:GLU:HG2	1:D:275:MET:HE3	1.96	0.46
1:D:326:LYS:HB3	1:D:370:LYS:HB2	1.98	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: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:B:215:LEU:HD23	1:B:215:LEU:C	2.37	0.45
1:B:311:MET:HE1	1:B:350:VAL:HG11	1.99	0.45
1:D:372:VAL:CG1	1:D:373:THR:N	2.79	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:MET:HE1	1:A:269:LEU:HD23	1.97	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:D:290:VAL:HG13	1:D:311:MET:HE1	1.99	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:D:165:LYS:O	1:D:166:ASN:C	2.53	0.44
1:A:159:ALA:O	1:A:163:THR:HG23	2.17	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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:272:GLU:HA	1:D:275:MET:HE3	2.00	0.42
1:A:215:LEU:HD11	1:A:372:VAL:HG13	2.00	0.42
1:B:311:MET:CE	1:B:350:VAL:HG11	2.49	0.42
1:C:377:ARG:C	1:C:384:ILE:HD11	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ALA:HB1	1:C:82:MET:HE1	2.00	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:205:LYS:HA	1:A:205:LYS:HD3	1.83	0.42
1:D:88:THR:HA	1:D:91:LYS:HZ2	1.84	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:C:266:MET:HE2	1:C:266:MET:HA	2.02	0.42
1:A:227:HIS:HD2	1:A:229:ARG:HB2	1.84	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:C:445:LYS:C	1:C:448:PRO:HD2	2.40	0.41
1:A:257:ILE:HB	1:B:255:ALA:HB2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:271:GLN:O	1:B:275:MET:HE2	2.20	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:B:163:THR:HB	1:B:171:LYS:HZ1	1.80	0.41
1:B:290:VAL:HG13	1:B:311:MET:CE	2.51	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:266:MET:CE	1:A:269:LEU:HD23	2.51	0.41
1:A:271:GLN:HG3	1:A:275:MET:CE	2.50	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:D:311:MET:HE1	1:D:350:VAL:HG11	2.02	0.40
1:A:271:GLN:HG3	1:A:275:MET:HE2	2.02	0.40
1:A:463:LEU:HD13	1:A:463:LEU:HA	1.90	0.40
1:B:110:LYS:HA	1:B:110:LYS:HE2	2.02	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
1:D:446:ILE:O	1:D:450:THR:CG2	2.53	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	516/548 (94%)	504 (98%)	10 (2%)	2 (0%)	34	42
1	B	516/548 (94%)	503 (98%)	10 (2%)	3 (1%)	25	31
1	C	516/548 (94%)	500 (97%)	12 (2%)	4 (1%)	19	23
1	D	516/548 (94%)	502 (97%)	11 (2%)	3 (1%)	25	31
All	All	2064/2192 (94%)	2009 (97%)	43 (2%)	12 (1%)	25	31

All (12) Ramachandran outliers are listed below:

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

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%)	398 (94%)	25 (6%)	19	27
1	B	423/441 (96%)	399 (94%)	24 (6%)	20	28
1	C	423/441 (96%)	400 (95%)	23 (5%)	22	30
1	D	423/441 (96%)	394 (93%)	29 (7%)	15	20
All	All	1692/1764 (96%)	1591 (94%)	101 (6%)	19	26

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
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	229	ARG
1	A	238	LYS
1	A	258	ASN
1	A	269	LEU
1	A	305	LEU
1	A	358	GLU
1	A	372	VAL
1	A	375	LEU
1	A	377	ARG
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

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Mol	Chain	Res	Type
1	A	516	LEU
1	B	14	GLU
1	B	30	LEU
1	B	82	MET
1	B	125	THR
1	B	147	ASP
1	B	154	LEU
1	B	155	LEU
1	B	169	SER
1	B	211	GLU
1	B	229	ARG
1	B	241	LEU
1	B	269	LEU
1	B	305	LEU
1	B	368	ASN
1	B	375	LEU
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
1	C	30	LEU
1	C	82	MET
1	C	107	LEU
1	C	153	THR
1	C	154	LEU
1	C	155	LEU
1	C	241	LEU
1	C	269	LEU
1	C	305	LEU
1	C	315	ARG
1	C	367	LYS
1	C	375	LEU
1	C	377	ARG
1	C	435	LEU
1	C	446	ILE
1	C	450	THR

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Mol	Chain	Res	Type
1	C	459	THR
1	C	463	LEU
1	C	483	GLU
1	C	490	LEU
1	C	498	LEU
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	147	ASP
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	269	LEU
1	D	305	LEU
1	D	367	LYS
1	D	375	LEU
1	D	377	ARG
1	D	380	THR
1	D	435	LEU
1	D	446	ILE
1	D	450	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 (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	75	GLN
1	A	76	HIS

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Mol	Chain	Res	Type
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	117	GLN
1	B	118	ASN
1	B	170	HIS
1	B	184	GLN
1	B	258	ASN
1	B	282	HIS
1	B	285	GLN
1	B	303	HIS
1	B	335	ASN
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	227	HIS
1	C	282	HIS
1	C	285	GLN
1	C	303	HIS
1	C	335	ASN
1	C	368	ASN
1	C	428	GLN
1	C	503	GLN
1	D	17	GLN
1	D	28	ASN
1	D	75	GLN
1	D	76	HIS

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Mol	Chain	Res	Type
1	D	89	GLN
1	D	117	GLN
1	D	118	ASN
1	D	170	HIS
1	D	184	GLN
1	D	227	HIS
1	D	282	HIS
1	D	285	GLN
1	D	303	HIS
1	D	335	ASN
1	D	368	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	D	4528	2	29,33,33	1.57	8 (27%)	31,52,52	1.50	5 (16%)
3	ANP	C	3528	2	29,33,33	1.57	8 (27%)	31,52,52	1.49	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	B	2528	2	29,33,33	1.53	8 (27%)	31,52,52	1.53	5 (16%)
3	ANP	A	1528	2	29,33,33	1.62	8 (27%)	31,52,52	1.46	5 (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
3	ANP	D	4528	2	-	4/14/38/38	0/3/3/3
3	ANP	C	3528	2	-	4/14/38/38	0/3/3/3
3	ANP	B	2528	2	-	4/14/38/38	0/3/3/3
3	ANP	A	1528	2	-	4/14/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1528	ANP	PB-O3A	3.65	1.63	1.59
3	D	4528	ANP	PB-O3A	3.42	1.63	1.59
3	A	1528	ANP	PB-O2B	-3.36	1.47	1.56
3	D	4528	ANP	PB-O2B	-3.32	1.47	1.56
3	B	2528	ANP	PB-O2B	-3.31	1.47	1.56
3	C	3528	ANP	PB-O2B	-3.30	1.47	1.56
3	B	2528	ANP	PB-O3A	2.98	1.62	1.59
3	C	3528	ANP	PG-O2G	-2.95	1.48	1.56
3	C	3528	ANP	PB-O3A	2.94	1.62	1.59
3	D	4528	ANP	PG-O2G	-2.88	1.49	1.56
3	B	2528	ANP	PG-O2G	-2.83	1.49	1.56
3	A	1528	ANP	PG-O2G	-2.79	1.49	1.56
3	A	1528	ANP	PG-O3G	-2.72	1.49	1.56
3	C	3528	ANP	O4'-C1'	2.71	1.44	1.41
3	C	3528	ANP	C2-N3	2.70	1.36	1.32
3	C	3528	ANP	PG-O3G	-2.67	1.49	1.56
3	B	2528	ANP	C2-N3	2.63	1.36	1.32
3	A	1528	ANP	O4'-C1'	2.62	1.44	1.41
3	D	4528	ANP	C2-N3	2.55	1.36	1.32
3	D	4528	ANP	O4'-C1'	2.53	1.44	1.41
3	B	2528	ANP	O4'-C1'	2.50	1.44	1.41
3	B	2528	ANP	PG-O3G	-2.46	1.50	1.56
3	A	1528	ANP	C2-N3	2.44	1.36	1.32
3	D	4528	ANP	PG-O3G	-2.41	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3528	ANP	PG-O1G	2.32	1.49	1.46
3	D	4528	ANP	C4-N3	2.27	1.38	1.35
3	A	1528	ANP	C4-N3	2.23	1.38	1.35
3	C	3528	ANP	C4-N3	2.20	1.38	1.35
3	B	2528	ANP	C4-N3	2.18	1.38	1.35
3	A	1528	ANP	PG-O1G	2.15	1.49	1.46
3	B	2528	ANP	PG-O1G	2.13	1.49	1.46
3	D	4528	ANP	PG-O1G	2.03	1.49	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1528	ANP	O2B-PB-O1B	4.67	119.71	109.92
3	B	2528	ANP	O2B-PB-O1B	4.57	119.50	109.92
3	D	4528	ANP	O2B-PB-O1B	4.50	119.37	109.92
3	C	3528	ANP	O2B-PB-O1B	4.28	118.90	109.92
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	C3'-C2'-C1'	2.77	105.15	100.98
3	C	3528	ANP	C5-C6-N6	2.76	124.54	120.35
3	A	1528	ANP	C5-C6-N6	2.74	124.51	120.35
3	B	2528	ANP	C5-C6-N6	2.70	124.45	120.35
3	D	4528	ANP	C5-C6-N6	2.65	124.38	120.35
3	C	3528	ANP	O1G-PG-N3B	-2.64	107.88	111.77
3	A	1528	ANP	O4'-C1'-C2'	-2.39	103.44	106.93
3	A	1528	ANP	C3'-C2'-C1'	2.25	104.36	100.98
3	B	2528	ANP	O4'-C1'-C2'	-2.25	103.64	106.93
3	D	4528	ANP	O4'-C1'-C2'	-2.22	103.68	106.93
3	A	1528	ANP	O1B-PB-N3B	-2.21	108.51	111.77
3	B	2528	ANP	C3'-C2'-C1'	2.20	104.30	100.98
3	D	4528	ANP	C3'-C2'-C1'	2.20	104.29	100.98
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
3	A	1528	ANP	PA-O3A-PB-O1B
3	A	1528	ANP	PA-O3A-PB-O2B
3	B	2528	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
3	B	2528	ANP	PG-N3B-PB-O1B
3	B	2528	ANP	PA-O3A-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-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-O1B
3	D	4528	ANP	PA-O3A-PB-O2B

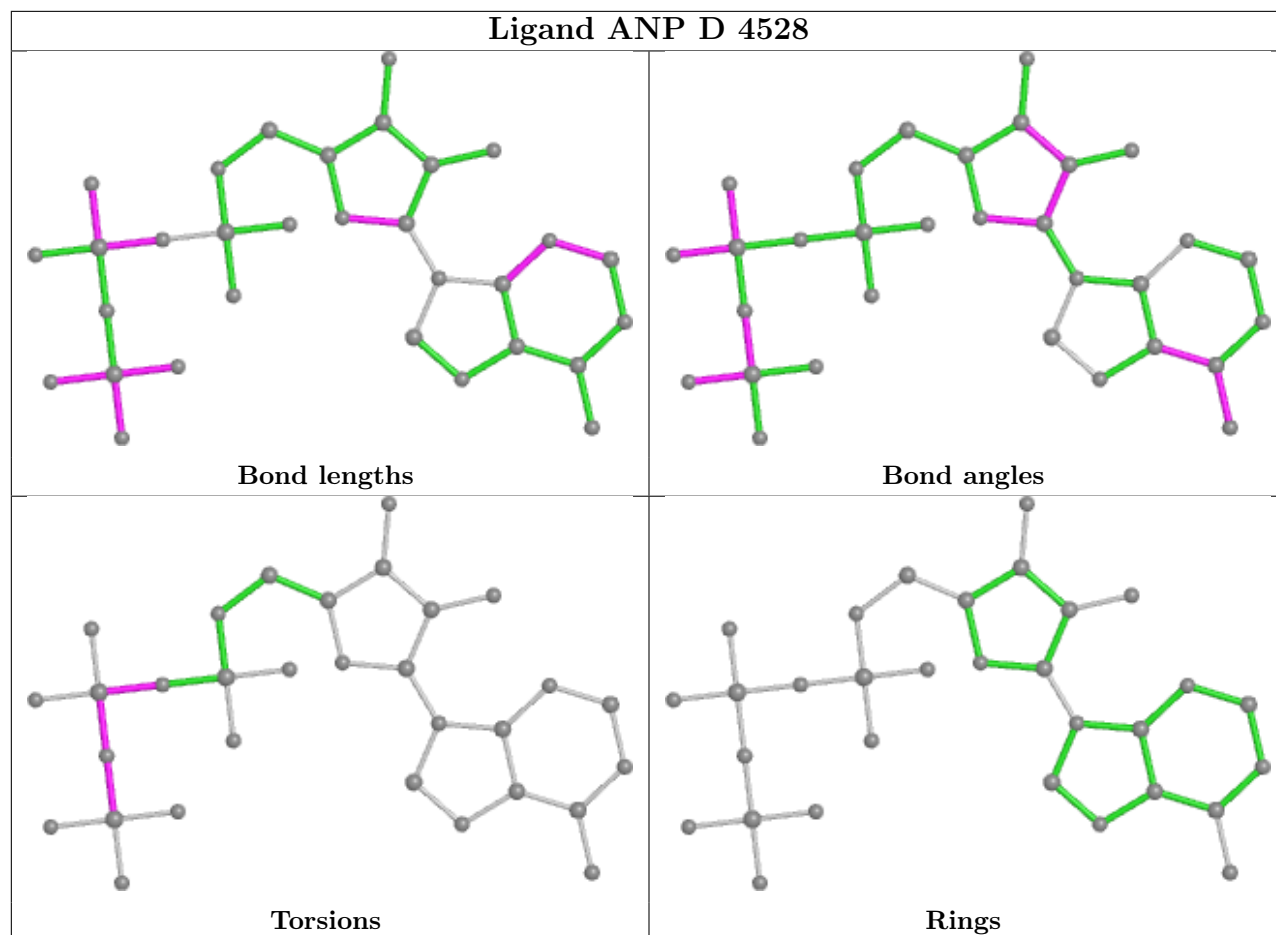
There are no ring outliers.

4 monomers are involved in 8 short contacts:

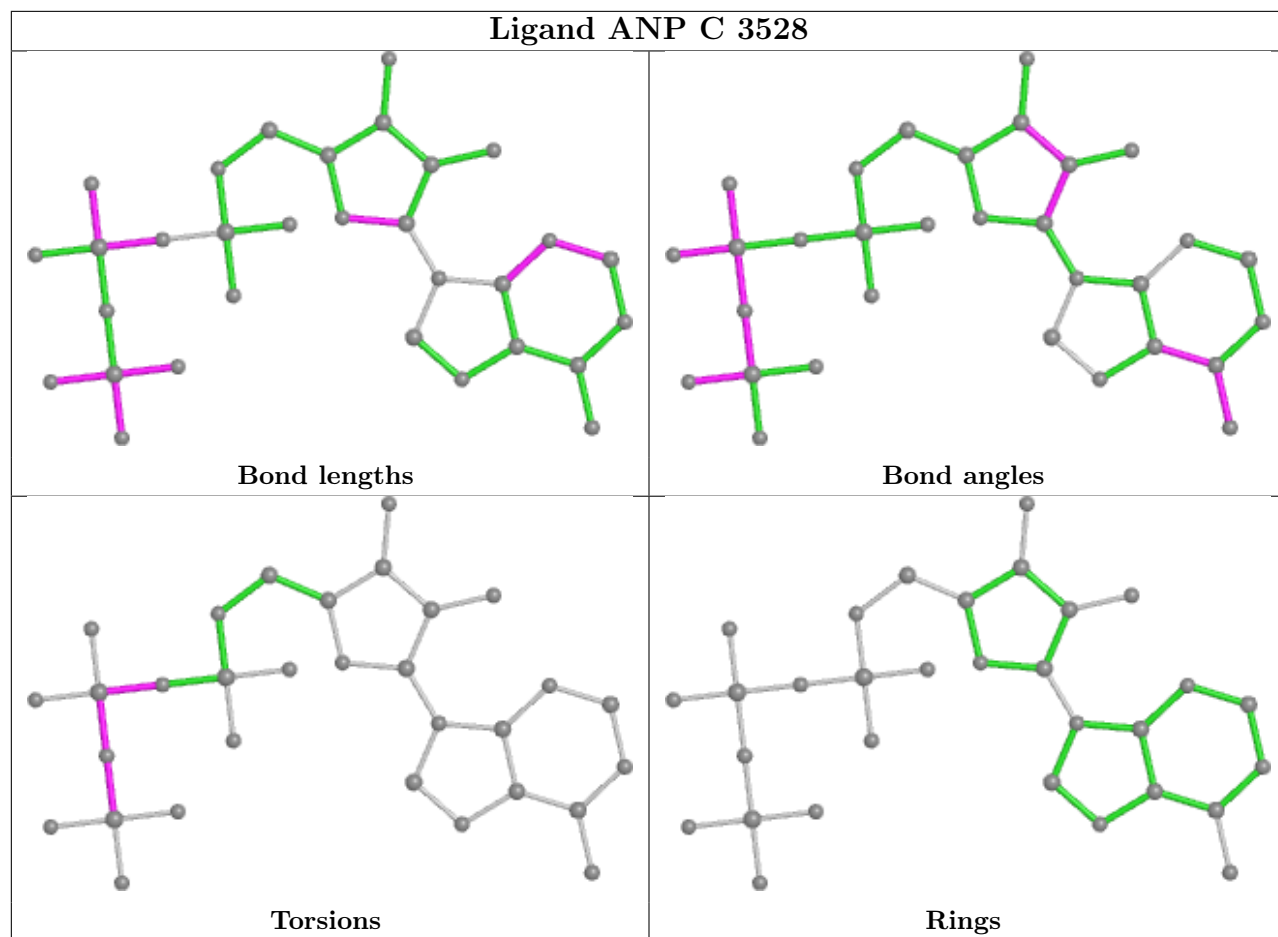
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4528	ANP	2	0
3	C	3528	ANP	2	0
3	B	2528	ANP	2	0
3	A	1528	ANP	2	0

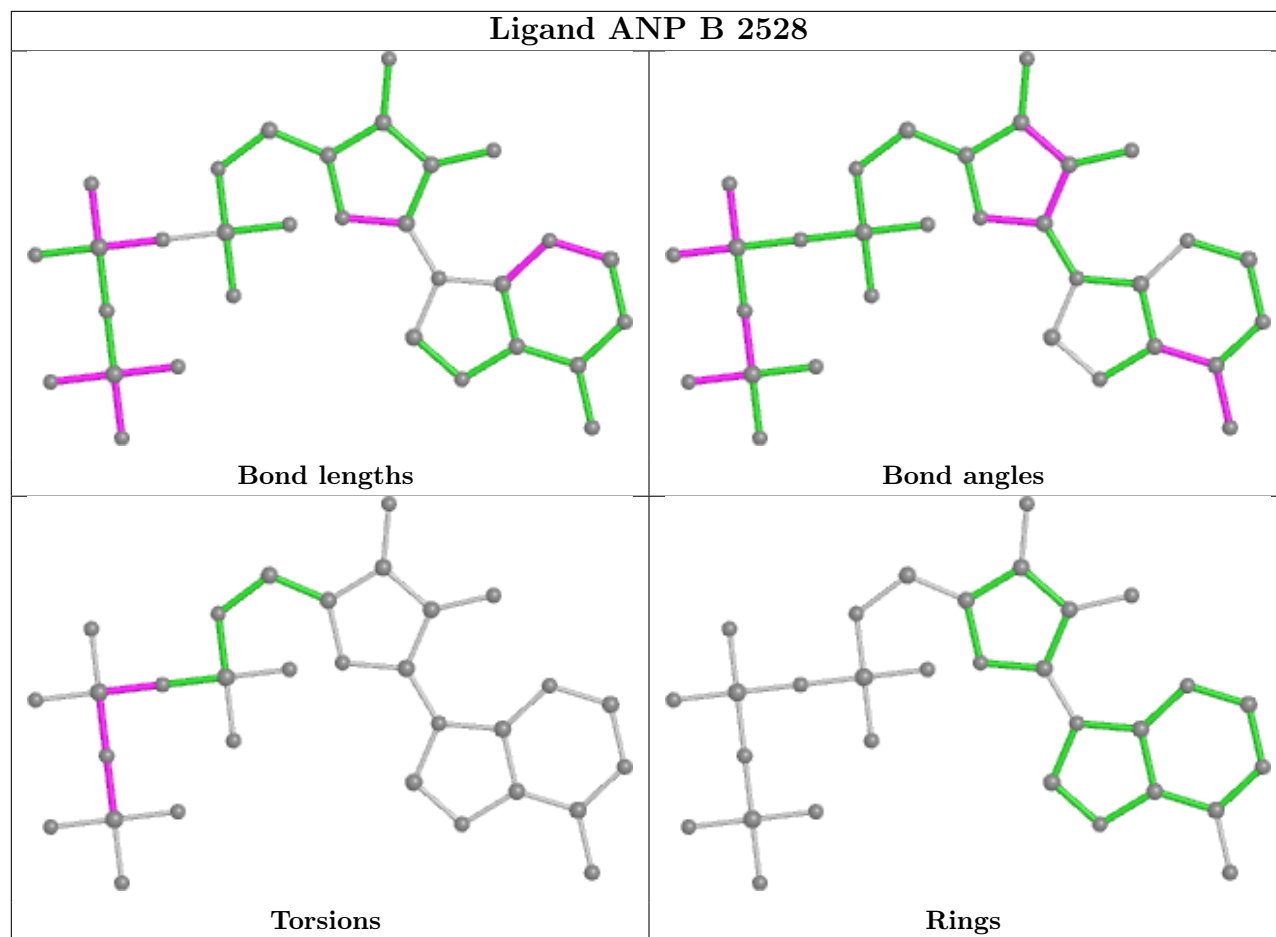
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

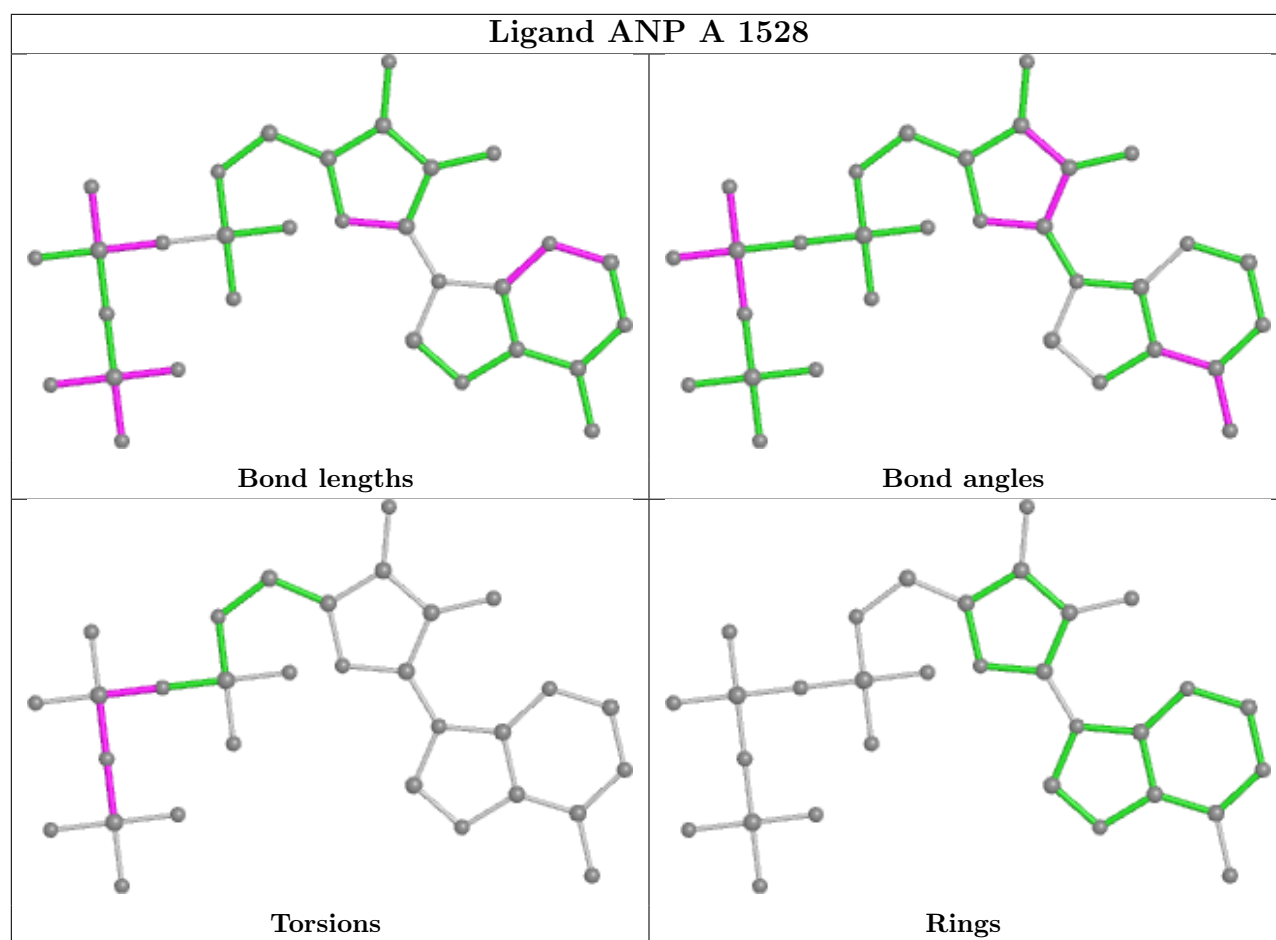
Ligand ANP D 4528



Ligand ANP C 3528







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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

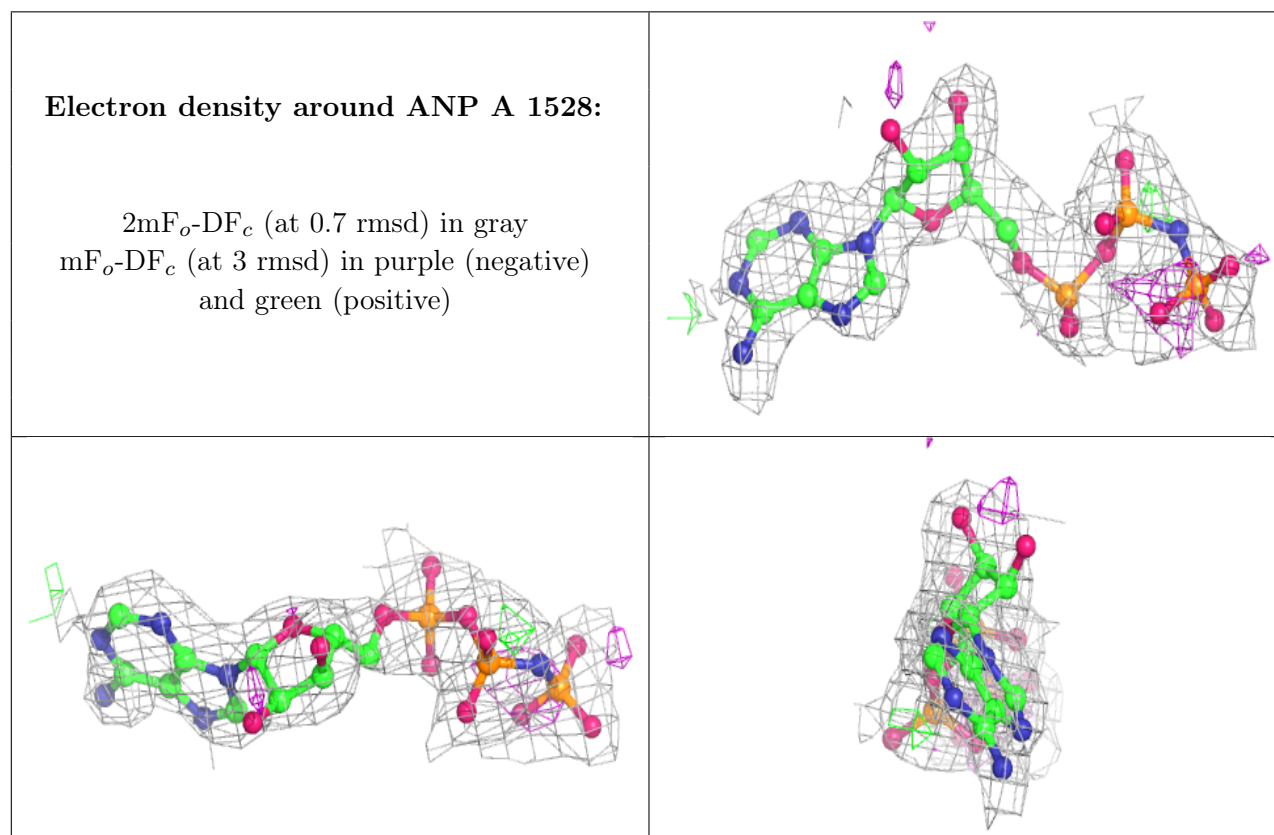
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

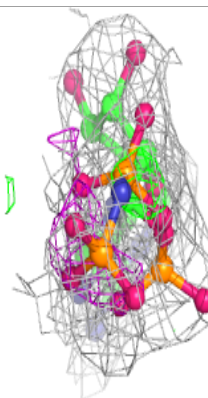
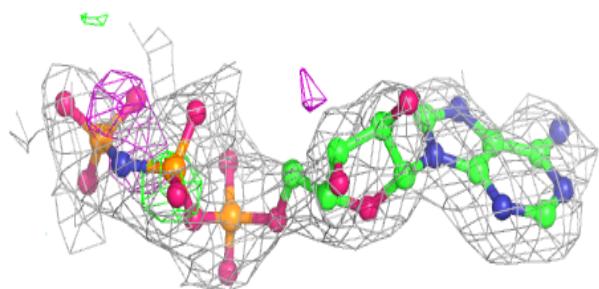
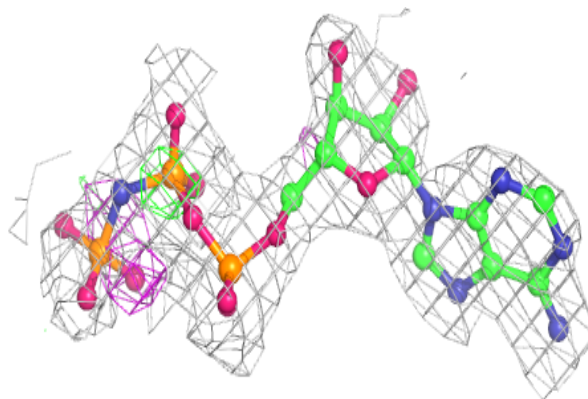
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

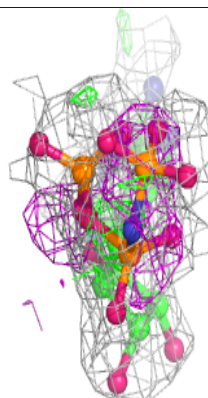
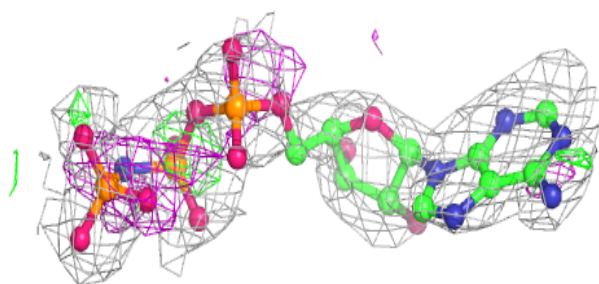
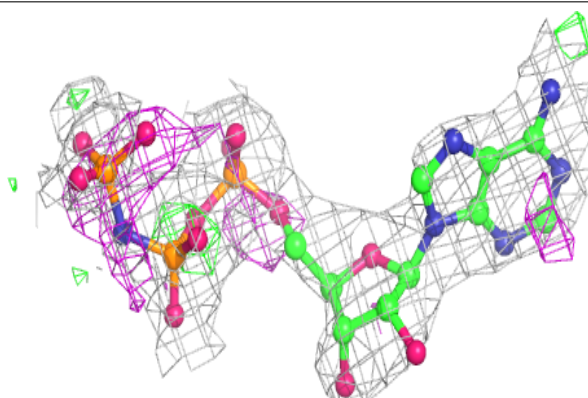


Electron density around ANP B 2528:

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

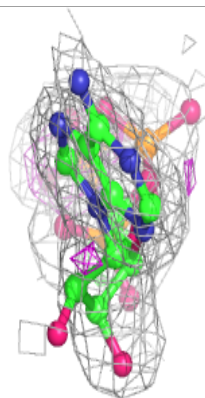
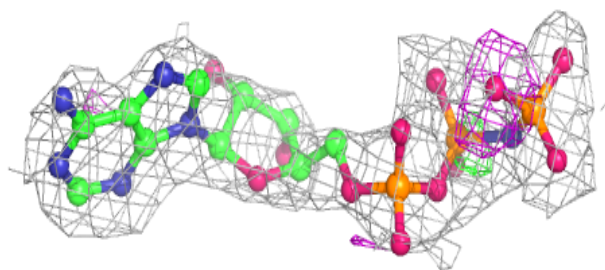
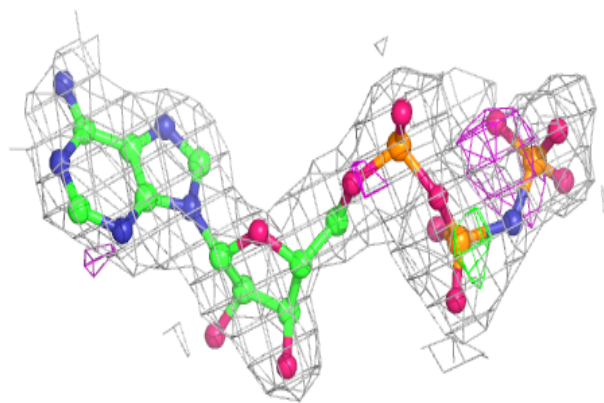
**Electron density around ANP C 3528:**

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



Electron density around ANP 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.