Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:06 pm BST

PDB ID	:	5EAW
Title	:	Crystal structure of Dna2 nuclease-helicase
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Deposited on	:	2015-10-17
Resolution	:	3.00 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:

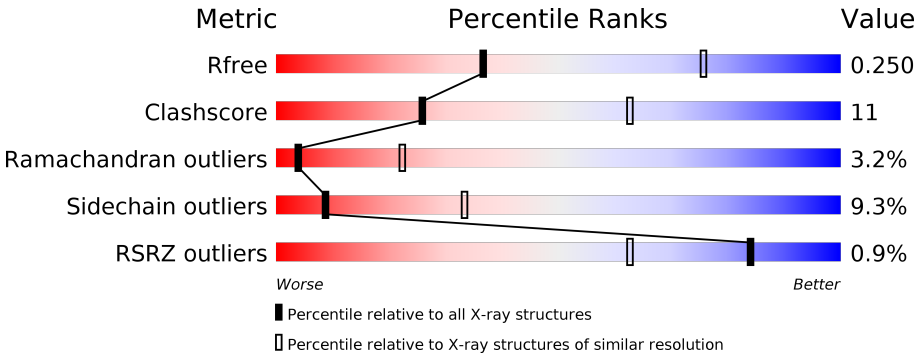
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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 <=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	1056	% 70% 24%
1	B	1056	% 70% 25%

2 Entry composition

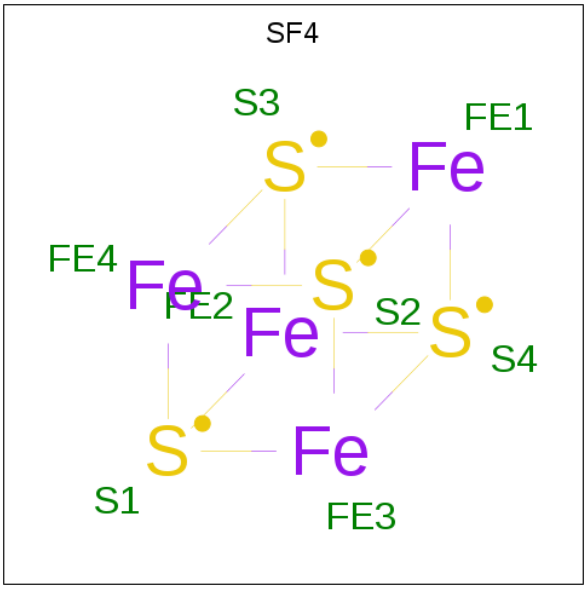
There are 3 unique types of molecules in this entry. The entry contains 16612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA replication ATP-dependent helicase/nuclease DNA2.

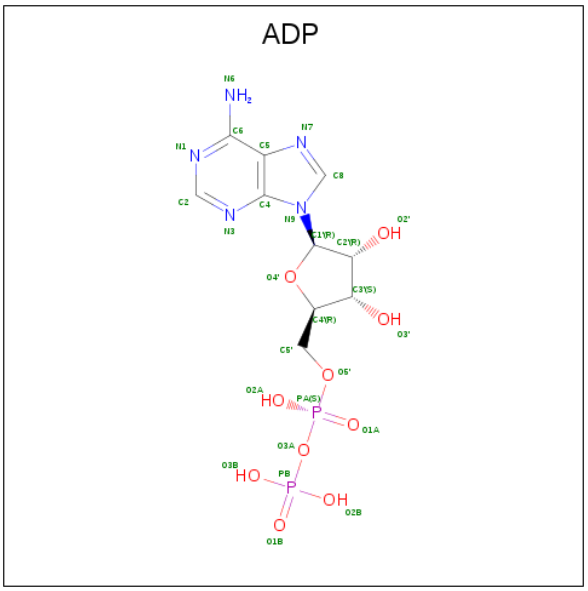
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1046	Total	C	N	O	S	0	0	0
			8271	5222	1456	1548	45			
1	B	1046	Total	C	N	O	S	0	0	0
			8271	5222	1456	1548	45			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Fe	S		0	0
			8	4	4			
2	B	1	Total	Fe	S		0	0
			8	4	4			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



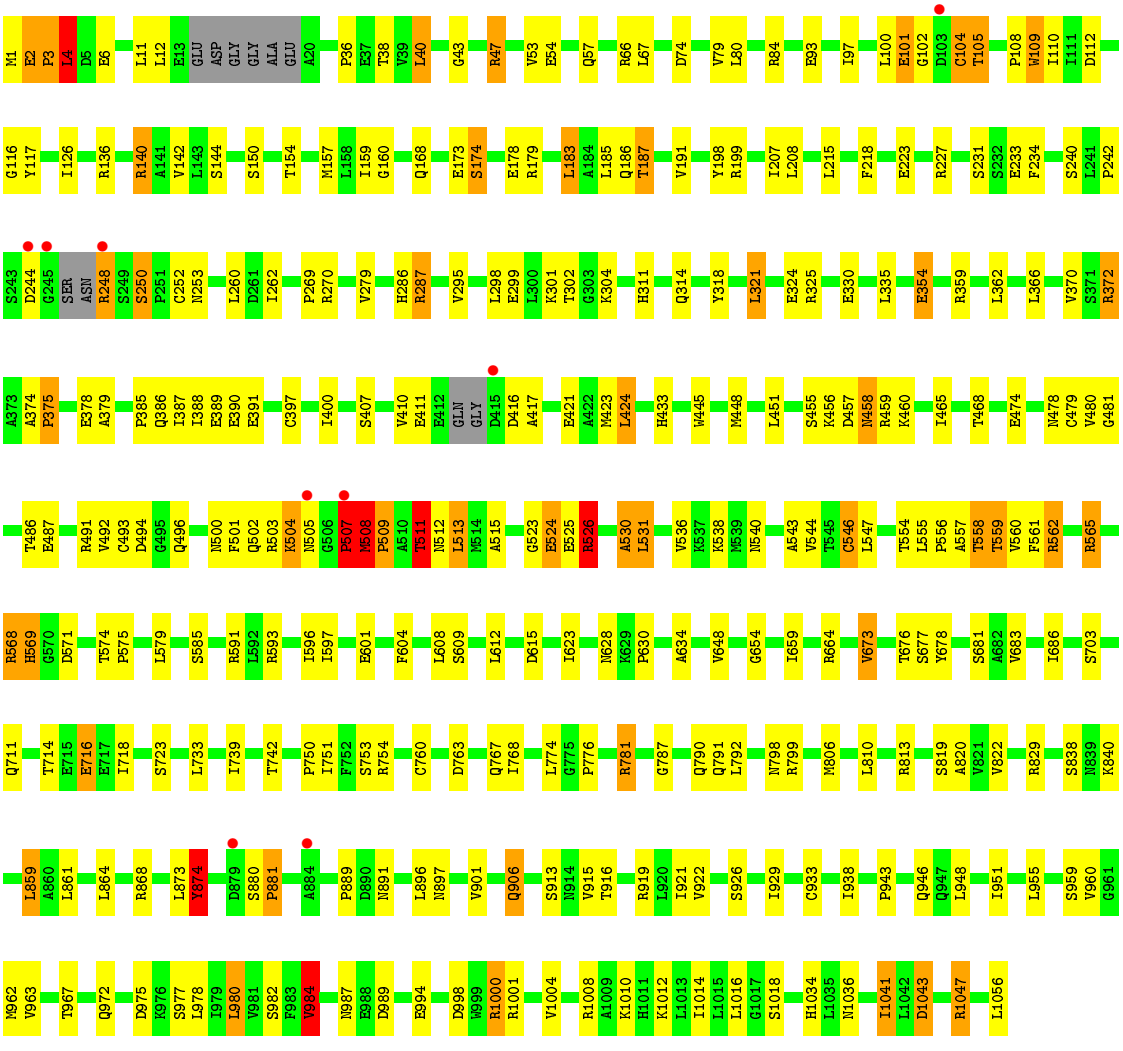
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots (i)

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

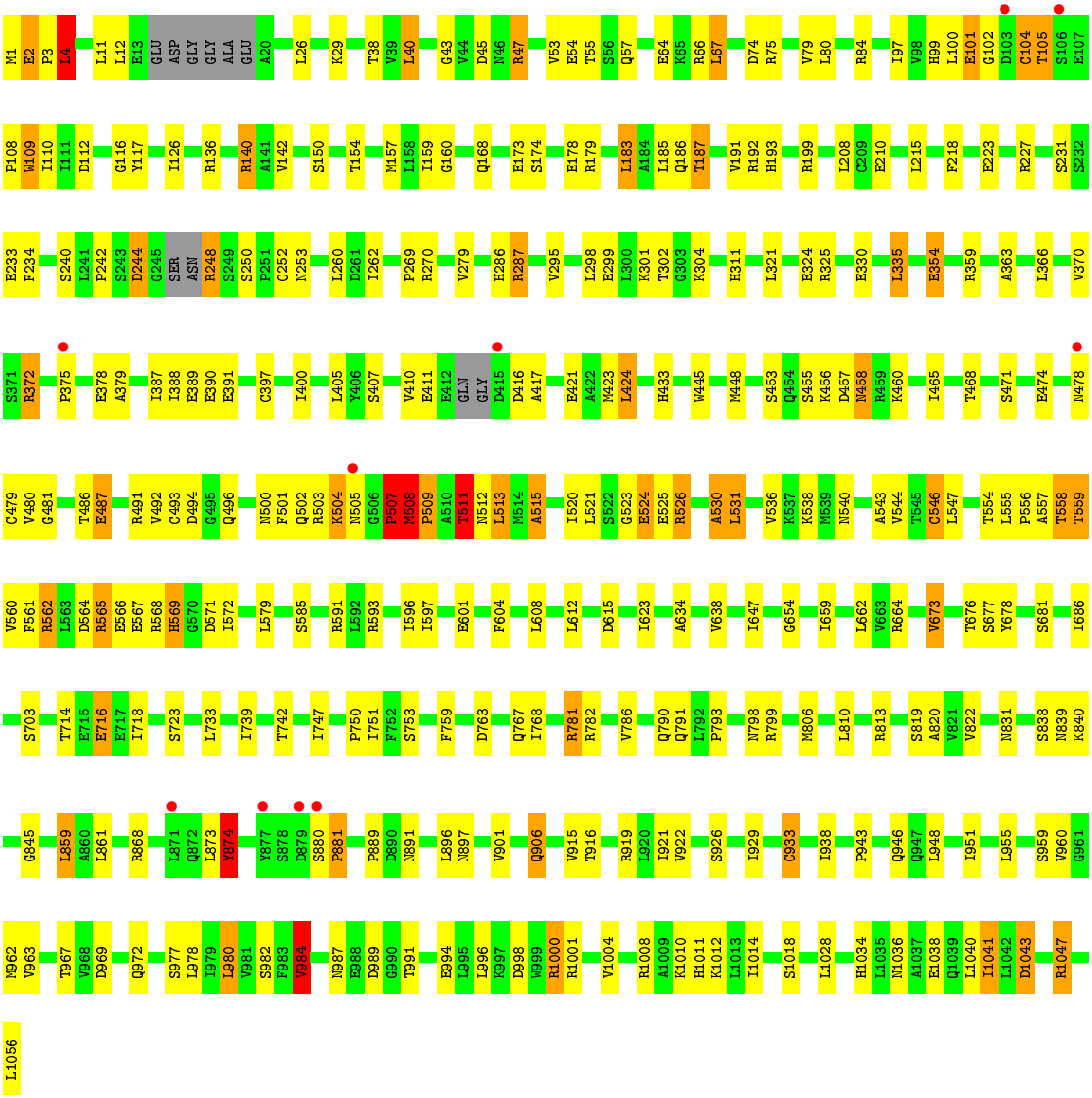
- Molecule 1: DNA replication ATP-dependent helicase/nuclease DNA2

Chain A:



- Molecule 1: DNA replication ATP-dependent helicase/nuclease DNA2

Chain B:


M1 E2 P3 L4 L11 L12 E13 GLU ASP GLY GLY ALA GLU A20 L26 K29 T38 V39 L40 G43 V44 D45 N46 R47 V53 E54 T55 S56 Q57 E64 K65 R66 L67 D74 R75 V79 L80 R84 I97 V98 H99 L100 E101 G102 D103 C104 T105 S106 E107
P108 W109 I110 I111 D112 G116 Y117 I126 R136 R140 A141 V142 S150 T154 M157 L158 I159 G160 Q168 E173 S174 E178 R179 L183 A184 L185 Q186 T187 V191 R192 H193 R199 L208 C209 E210 L215 F218 E223 R227 S231 S232
E233 F234 S240 L241 P242 S243 D244 G245 SER ASN R248 S249 S250 P251 C252 N253 L260 D261 I262 P269 R270 V279 H286 R287 V295 L298 E299 L300 K301 T302 G303 K304 H311 L321 E324 R325 E330 L335 E384 R359 A363 L366 V370
S371 R372 P375 E378 A379 I387 I388 E389 E390 E391 C397 I400 L405 Y406 S407 V410 E411 E412 GLN GLY D415 D416 A417 E421 A422 M423 L424 H433 W445 M448 S453 Q454 S455 K456 D457 N458 R459 K460 I465 T468 S471 E474 N478
C479 V480 G481 T486 E487 R491 V492 C493 D494 G495 Q496 N500 P501 Q502 R503 K504 N505 G506 P507 M508 P509 A510 T511 N512 L513 M514 A515 I520 L521 S522 G523 E524 E525 R526 A530 L531 V536 K537 K538 M539 N540 A543 V544 T545 C546 L547 T554 L555 P556 A557 T558 T559
V560 F561 R562 L563 D564 R565 E566 E567 R568 H569 G570 D571 I572 L579 S585 R591 L592 R593 I596 I597 E601 F604 L608 L612 D615 I623 A634 V638 I647 G654 I659 L662 V663 R664 V673 T676 S677 Y678 S681 I686
S703 T714 E715 E716 E717 I718 S723 L733 I739 T742 I747 P750 I751 F752 S753 F759 D763 Q767 I768 R781 R782 V786 Q790 Q791 L792 P793 N798 R799 M806 L810 R813 S819 A820 V821 V822 N831 S838 N839 K840
G845 L859 A860 I861 R868 L871 Q872 I873 Y874 Y877 S878 D879 S880 P881 P889 D890 N891 L896 N897 V901 Q906 V915 T916 R919 L920 I921 V922 S926 I929 G933 I938 P943 Q946 Q947 L948 I951 L955 S959 V960 G961
M962 V963 T967 V968 D969 Q972 S977 L978 I979 L980 V981 S982 F983 V984 N987 E988 D989 G990 T991 E994 L995 L996 K997 D998 W999 R1000 R1001 V1004 R1008 A1009 K1010 H1011 K1012 L1013 I1014 S1018 L1028 H1034 L1035 N1036 A1037 E1038 Q1039 L1040 I1041 L1042 D1043 R1047
L1056

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	120.90Å 148.60Å 170.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.31 – 2.98	Depositor EDS
% Data completeness (in resolution range)	89.2 (50.00-3.00) 88.4 (49.31-2.98)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.209 , 0.247 0.215 , 0.250	Depositor DCC
R_{free} test set	1555 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å^2)	48.3	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16612	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1691e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SF4, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.57	0/8421	0.83	5/11387 (0.0%)
1	B	0.56	0/8421	0.83	4/11387 (0.0%)
All	All	0.56	0/16842	0.83	9/22774 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
All	All	0	6

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4	LEU	CA-CB-CG	7.61	132.81	115.30
1	B	4	LEU	CA-CB-CG	7.15	131.75	115.30
1	A	12	LEU	CA-CB-CG	5.94	128.97	115.30
1	B	12	LEU	CA-CB-CG	5.91	128.90	115.30
1	A	774	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	526	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	11	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	11	LEU	CA-CB-CG	5.10	127.02	115.30
1	B	67	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	CYS	Peptide
1	A	507	PRO	Peptide
1	A	508	MET	Peptide
1	B	104	CYS	Peptide
1	B	507	PRO	Peptide
1	B	508	MET	Peptide

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	8271	0	8411	177	0
1	B	8271	0	8411	177	0
2	A	8	0	0	0	0
2	B	8	0	0	1	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
All	All	16612	0	16846	352	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (352) 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:B:458:ASN:HB2	1:B:569:HIS:HB3	1.53	0.90
1:A:511:THR:H	1:A:513:LEU:HD21	1.37	0.89
1:A:43:GLY:H	1:A:105:THR:HG21	1.41	0.86
1:B:511:THR:H	1:B:513:LEU:HD21	1.38	0.85
1:B:183:LEU:O	1:B:187:THR:HG23	1.77	0.85
1:B:43:GLY:H	1:B:105:THR:HG21	1.41	0.84
1:B:154:THR:HG22	1:B:157:MET:HG3	1.63	0.81
1:A:458:ASN:HB2	1:A:569:HIS:HB3	1.62	0.81
1:A:183:LEU:O	1:A:187:THR:HG23	1.80	0.79
1:A:298:LEU:HD11	1:A:335:LEU:HB2	1.68	0.75
1:B:799:ARG:HH22	1:B:994:GLU:HG3	1.51	0.75
1:A:154:THR:HG22	1:A:157:MET:HG3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LEU:HD11	1:B:335:LEU:HB2	1.69	0.74
1:B:493:CYS:O	1:B:496:GLN:HG2	1.89	0.72
1:A:593:ARG:HG2	1:A:597:ILE:HD12	1.72	0.72
1:B:596:ILE:O	1:B:813:ARG:NH1	2.23	0.72
1:A:493:CYS:O	1:A:496:GLN:HG2	1.89	0.72
1:B:508:MET:HB3	1:B:509:PRO:HD3	1.71	0.72
1:B:2:GLU:HB2	1:B:3:PRO:HD3	1.72	0.71
1:B:478:ASN:HB3	1:B:565:ARG:HG2	1.72	0.71
1:B:593:ARG:HG2	1:B:597:ILE:HD12	1.72	0.71
1:B:891:ASN:O	1:B:1012:LYS:NZ	2.24	0.71
1:B:433:HIS:CG	1:B:585:SER:HB3	2.27	0.70
1:A:596:ILE:O	1:A:813:ARG:NH1	2.24	0.70
1:A:714:THR:HG22	1:A:716:GLU:H	1.57	0.70
1:A:508:MET:HB3	1:A:509:PRO:HD3	1.73	0.70
1:B:526:ARG:HG2	1:B:526:ARG:HH11	1.58	0.69
1:A:478:ASN:HB3	1:A:565:ARG:CG	2.23	0.68
1:A:511:THR:N	1:A:513:LEU:HD21	2.08	0.68
1:B:714:THR:HG22	1:B:716:GLU:H	1.58	0.68
1:B:84:ARG:HH21	1:B:110:ILE:HG21	1.59	0.67
1:A:487:GLU:HG3	1:A:500:ASN:HB3	1.75	0.67
1:A:799:ARG:HH22	1:A:994:GLU:HG3	1.60	0.66
1:A:503:ARG:HH11	1:A:503:ARG:HB2	1.61	0.66
1:B:503:ARG:HH11	1:B:503:ARG:HB2	1.60	0.66
1:A:109:TRP:HB3	1:A:110:ILE:HD12	1.77	0.65
1:A:2:GLU:HB2	1:A:3:PRO:HD3	1.79	0.65
1:A:901:VAL:HG23	1:A:1047:ARG:HB3	1.77	0.65
1:A:335:LEU:HD12	1:A:335:LEU:O	1.96	0.65
1:A:880:SER:N	1:A:881:PRO:HD2	2.13	0.64
1:B:102:GLY:HA3	1:B:116:GLY:HA2	1.80	0.64
1:B:511:THR:N	1:B:513:LEU:HD21	2.12	0.64
1:A:478:ASN:HB3	1:A:565:ARG:HG2	1.79	0.64
1:B:487:GLU:HG3	1:B:500:ASN:HB3	1.79	0.63
1:B:880:SER:N	1:B:881:PRO:HD2	2.13	0.63
1:A:526:ARG:HG2	1:A:526:ARG:HH11	1.62	0.63
1:A:102:GLY:CA	1:A:117:TYR:H	2.11	0.63
1:B:407:SER:O	1:B:411:GLU:HB3	1.99	0.63
1:B:102:GLY:CA	1:B:117:TYR:H	2.12	0.62
1:A:654:GLY:HA2	3:A:1102:ADP:O2B	1.98	0.62
1:A:84:ARG:HH21	1:A:110:ILE:HG21	1.65	0.62
1:A:767:GLN:OE1	1:A:972:GLN:NE2	2.32	0.62
1:B:53:VAL:HG22	1:B:67:LEU:HD22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLU:HB3	1:B:608:LEU:HD21	1.82	0.61
1:A:102:GLY:HA3	1:A:116:GLY:HA2	1.83	0.61
1:B:372:ARG:HH21	1:B:379:ALA:HB2	1.66	0.61
1:B:511:THR:H	1:B:513:LEU:CD2	2.13	0.61
1:A:524:GLU:HG3	1:A:525:GLU:H	1.66	0.61
1:A:448:MET:HB3	1:A:806:MET:HG3	1.82	0.61
1:B:901:VAL:HG23	1:B:1047:ARG:HB3	1.83	0.61
1:B:524:GLU:HB3	1:B:560:VAL:HB	1.82	0.61
1:A:524:GLU:HB3	1:A:560:VAL:HB	1.81	0.60
1:B:465:ILE:HA	1:B:562:ARG:NH1	2.17	0.60
1:A:511:THR:H	1:A:513:LEU:CD2	2.11	0.60
1:B:455:SER:OG	1:B:798:ASN:HB2	2.01	0.60
1:B:526:ARG:NH1	1:B:526:ARG:HG2	2.17	0.60
1:B:335:LEU:HD12	1:B:335:LEU:O	2.02	0.60
1:B:1000:ARG:HB2	1:B:1000:ARG:HH11	1.66	0.59
1:B:301:LYS:HZ3	1:B:311:HIS:HD2	1.50	0.59
1:B:524:GLU:HG3	1:B:525:GLU:H	1.67	0.59
1:B:2:GLU:HB2	1:B:3:PRO:CD	2.32	0.59
1:B:433:HIS:CD2	1:B:585:SER:HB3	2.37	0.59
1:B:102:GLY:CA	1:B:116:GLY:HA2	2.33	0.59
1:B:388:ILE:HD12	1:B:390:GLU:HB3	1.84	0.58
1:A:840:LYS:HD2	1:A:1034:HIS:CD2	2.39	0.58
1:A:891:ASN:O	1:A:1012:LYS:NZ	2.35	0.58
1:A:102:GLY:CA	1:A:116:GLY:HA2	2.33	0.58
1:A:227:ARG:HG2	1:A:234:PHE:CE1	2.39	0.58
1:A:526:ARG:HG2	1:A:526:ARG:NH1	2.19	0.58
1:B:227:ARG:HG2	1:B:234:PHE:CE1	2.39	0.57
1:A:240:SER:HA	1:A:248:ARG:HB3	1.86	0.57
1:B:109:TRP:HB3	1:B:110:ILE:HD12	1.85	0.57
1:B:503:ARG:HG2	1:B:504:LYS:O	2.04	0.57
1:A:465:ILE:HA	1:A:562:ARG:NH1	2.20	0.57
1:A:101:GLU:OE2	1:A:270:ARG:HD2	2.04	0.57
1:A:503:ARG:HG2	1:A:504:LYS:O	2.04	0.57
1:B:520:ILE:HG23	1:B:564:ASP:HB2	1.87	0.56
1:B:387:ILE:HG21	1:B:423:MET:HG2	1.86	0.56
1:B:767:GLN:OE1	1:B:972:GLN:NE2	2.39	0.56
1:A:524:GLU:CG	1:A:525:GLU:H	2.18	0.56
1:B:242:PRO:HG2	1:B:330:GLU:HG2	1.87	0.56
1:A:1000:ARG:HB2	1:A:1000:ARG:HH11	1.70	0.56
1:A:231:SER:HA	1:A:234:PHE:HD2	1.69	0.56
1:A:929:ILE:HA	1:A:933:CYS:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:HH21	1:A:379:ALA:HB2	1.71	0.56
1:A:407:SER:O	1:A:411:GLU:HB3	2.06	0.56
1:B:948:LEU:HD11	1:B:967:THR:HG23	1.88	0.56
1:B:673:VAL:HG13	1:B:739:ILE:HG12	1.86	0.56
1:B:354:GLU:OE2	1:B:354:GLU:HA	2.05	0.55
1:B:101:GLU:OE2	1:B:270:ARG:HD2	2.07	0.55
1:B:458:ASN:CB	1:B:569:HIS:HB3	2.33	0.55
1:A:325:ARG:HH22	1:A:531:LEU:H	1.53	0.55
1:A:530:ALA:O	1:A:531:LEU:HB2	2.07	0.55
1:A:433:HIS:CG	1:A:585:SER:HB3	2.42	0.55
1:A:474:GLU:HB3	1:A:479:CYS:O	2.06	0.55
1:B:977:SER:HA	1:B:1010:LYS:HB2	1.89	0.54
1:A:591:ARG:NH1	1:A:781:ARG:O	2.41	0.54
1:B:154:THR:HG23	1:B:157:MET:H	1.73	0.54
1:B:474:GLU:HB3	1:B:479:CYS:O	2.08	0.54
1:A:53:VAL:HG22	1:A:67:LEU:HD22	1.90	0.54
1:B:231:SER:HA	1:B:234:PHE:HD2	1.71	0.54
1:A:555:LEU:O	1:A:559:THR:OG1	2.23	0.54
1:B:142:VAL:HG13	1:B:366:LEU:HD23	1.90	0.54
1:B:325:ARG:HH22	1:B:531:LEU:H	1.55	0.54
1:A:262:ILE:HG22	1:A:279:VAL:HG13	1.90	0.54
1:B:524:GLU:CG	1:B:525:GLU:H	2.20	0.54
1:A:714:THR:HG22	1:A:716:GLU:N	2.23	0.54
1:B:873:LEU:O	1:B:874:TYR:HB2	2.08	0.53
1:A:2:GLU:HB2	1:A:3:PRO:CD	2.38	0.53
1:A:676:THR:HA	1:A:742:THR:O	2.08	0.53
1:A:478:ASN:HB3	1:A:565:ARG:HG3	1.90	0.53
1:A:387:ILE:HG21	1:A:423:MET:HG2	1.90	0.53
1:A:388:ILE:HD12	1:A:390:GLU:HB3	1.90	0.53
1:A:677:SER:HB3	1:A:763:ASP:HB3	1.91	0.53
1:A:242:PRO:HG2	1:A:330:GLU:HG2	1.90	0.53
1:A:906:GLN:OE1	1:A:915:VAL:HG23	2.08	0.53
1:B:262:ILE:HG22	1:B:279:VAL:HG13	1.90	0.53
1:B:508:MET:HB3	1:B:509:PRO:CD	2.38	0.53
1:B:906:GLN:OE1	1:B:915:VAL:HG23	2.08	0.53
1:B:638:VAL:HG11	1:B:662:LEU:HD11	1.91	0.52
1:B:922:VAL:HG22	1:B:955:LEU:HG	1.91	0.52
1:B:980:LEU:HD23	1:B:1014:ILE:HB	1.90	0.52
1:A:301:LYS:HZ3	1:A:311:HIS:HD2	1.55	0.52
1:A:38:THR:HG21	1:A:97:ILE:HG21	1.92	0.52
1:B:718:ILE:HG21	1:B:733:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:SER:OG	1:A:798:ASN:HB2	2.10	0.51
1:A:634:ALA:HA	1:A:822:VAL:HG11	1.92	0.51
1:A:354:GLU:HA	1:A:354:GLU:OE2	2.10	0.51
1:B:591:ARG:NH1	1:B:781:ARG:O	2.44	0.51
1:A:160:GLY:HA2	1:A:302:THR:HG21	1.92	0.51
1:A:948:LEU:HD11	1:A:967:THR:HG23	1.92	0.51
1:A:199:ARG:HG3	1:A:753:SER:OG	2.10	0.51
1:B:659:ILE:HG21	1:B:686:ILE:HD13	1.91	0.51
1:A:142:VAL:HG13	1:A:366:LEU:HD23	1.92	0.51
1:A:324:GLU:OE1	1:A:526:ARG:NH2	2.44	0.51
1:A:223:GLU:O	1:A:227:ARG:HB3	2.11	0.50
1:A:703:SER:HB3	1:A:714:THR:HG21	1.92	0.50
1:A:252:CYS:HB2	1:A:286:HIS:O	2.12	0.50
1:A:673:VAL:HG13	1:A:739:ILE:HG12	1.94	0.50
1:B:324:GLU:OE1	1:B:526:ARG:NH2	2.45	0.50
1:A:659:ILE:HG21	1:A:686:ILE:HD13	1.93	0.50
1:B:160:GLY:HA2	1:B:302:THR:HG21	1.93	0.50
1:A:301:LYS:HZ3	1:A:314:GLN:HE22	1.60	0.50
1:A:301:LYS:NZ	1:A:311:HIS:HD2	2.10	0.49
1:A:718:ILE:HG21	1:A:733:LEU:HD13	1.93	0.49
1:B:791:GLN:O	1:B:1000:ARG:HG2	2.12	0.49
1:A:154:THR:HG23	1:A:157:MET:H	1.77	0.49
1:B:677:SER:HB3	1:B:763:ASP:HB3	1.93	0.49
1:A:43:GLY:N	1:A:105:THR:HG21	2.20	0.49
1:B:38:THR:HG21	1:B:97:ILE:HG21	1.94	0.49
1:B:634:ALA:HA	1:B:822:VAL:HG11	1.93	0.49
1:B:540:ASN:HB2	1:B:543:ALA:H	1.77	0.49
1:A:569:HIS:C	1:A:571:ASP:N	2.66	0.49
1:A:678:TYR:HB2	1:A:768:ILE:HG12	1.95	0.49
1:B:199:ARG:HB2	1:B:750:PRO:HB3	1.93	0.49
1:B:929:ILE:HA	1:B:933:CYS:O	2.13	0.49
1:A:301:LYS:HD2	1:A:311:HIS:CD2	2.47	0.49
1:A:861:LEU:HD12	1:A:889:PRO:HG3	1.95	0.49
1:A:921:ILE:HG23	1:A:1016:LEU:HD22	1.95	0.48
1:A:790:GLN:O	1:A:1000:ARG:HG3	2.13	0.48
1:B:938:ILE:HG12	1:B:978:LEU:HD23	1.94	0.48
1:B:593:ARG:HG2	1:B:597:ILE:CD1	2.43	0.48
1:B:604:PHE:CZ	1:B:820:ALA:HA	2.48	0.48
1:B:240:SER:HA	1:B:248:ARG:HB3	1.96	0.48
1:B:678:TYR:HB2	1:B:768:ILE:HG12	1.94	0.48
1:A:508:MET:HB3	1:A:509:PRO:CD	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:VAL:HG23	1:B:513:LEU:HD22	1.96	0.48
1:A:929:ILE:HD13	1:A:960:VAL:CG1	2.44	0.48
1:B:325:ARG:NH2	1:B:531:LEU:H	2.12	0.48
1:B:676:THR:HA	1:B:742:THR:O	2.13	0.48
1:A:524:GLU:HG3	1:A:525:GLU:N	2.28	0.48
1:A:604:PHE:CZ	1:A:820:ALA:HA	2.48	0.47
1:B:253:ASN:HB2	1:B:286:HIS:HB2	1.96	0.47
1:A:922:VAL:HG22	1:A:955:LEU:HG	1.95	0.47
1:B:569:HIS:C	1:B:571:ASP:N	2.68	0.47
1:A:199:ARG:HB2	1:A:750:PRO:HB3	1.97	0.47
1:A:445:TRP:HB3	1:A:579:LEU:HD11	1.96	0.47
1:B:174:SER:HB3	1:B:179:ARG:HH11	1.79	0.47
1:A:421:GLU:HA	1:A:424:LEU:HB2	1.95	0.47
1:B:1036:ASN:OD1	1:B:1041:ILE:HG12	2.15	0.47
1:B:301:LYS:HD2	1:B:311:HIS:CD2	2.50	0.47
1:A:215:LEU:O	1:A:218:PHE:HB2	2.14	0.47
1:B:215:LEU:O	1:B:218:PHE:HB2	2.14	0.47
1:A:628:ASN:OD1	1:A:630:PRO:HD2	2.14	0.47
1:A:859:LEU:HD12	1:A:1012:LYS:HD2	1.97	0.47
1:A:980:LEU:HD23	1:A:1014:ILE:HB	1.95	0.47
1:B:252:CYS:HB2	1:B:286:HIS:O	2.15	0.47
1:B:260:LEU:CD1	1:B:295:VAL:HG22	2.45	0.47
1:B:536:VAL:HA	1:B:546:CYS:HB3	1.96	0.47
1:B:998:ASP:CG	1:B:1001:ARG:HG3	2.35	0.47
1:A:569:HIS:C	1:A:571:ASP:H	2.16	0.47
1:A:260:LEU:CD1	1:A:295:VAL:HG22	2.45	0.47
1:A:301:LYS:HZ3	1:A:314:GLN:NE2	2.13	0.47
1:B:301:LYS:NZ	1:B:311:HIS:HD2	2.12	0.47
1:B:919:ARG:HD2	1:B:1056:LEU:HD23	1.96	0.47
1:A:36:PRO:HD2	1:A:459:ARG:O	2.15	0.46
1:B:623:ILE:HD13	1:B:664:ARG:HB3	1.96	0.46
1:A:873:LEU:O	1:A:874:TYR:HB2	2.14	0.46
1:B:269:PRO:HD2	1:B:526:ARG:HH22	1.79	0.46
1:A:40:LEU:HA	1:A:47:ARG:O	2.16	0.46
1:A:767:GLN:CD	1:A:972:GLN:HE21	2.18	0.46
1:B:168:GLN:HB3	1:B:262:ILE:HD13	1.97	0.46
1:A:269:PRO:HD2	1:A:526:ARG:HH22	1.80	0.46
1:A:325:ARG:NH2	1:A:531:LEU:H	2.14	0.46
1:A:540:ASN:HB2	1:A:543:ALA:H	1.80	0.46
1:A:168:GLN:HB3	1:A:262:ILE:HD13	1.97	0.46
1:A:897:ASN:HB3	1:A:1043:ASP:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:SER:HB3	1:A:179:ARG:HH11	1.81	0.45
1:B:524:GLU:HG3	1:B:525:GLU:N	2.30	0.45
1:B:523:GLY:HA2	1:B:561:PHE:HA	1.97	0.45
1:B:421:GLU:HA	1:B:424:LEU:HB2	1.98	0.45
1:A:503:ARG:NH1	1:A:503:ARG:HB2	2.30	0.45
1:A:703:SER:O	1:A:711:GLN:NE2	2.49	0.45
1:A:929:ILE:CD1	1:A:960:VAL:HG11	2.46	0.45
1:B:793:PRO:HG3	1:B:1000:ARG:NH2	2.31	0.45
1:B:468:THR:O	1:B:562:ARG:NH2	2.49	0.45
1:A:524:GLU:CG	1:A:525:GLU:N	2.78	0.45
1:A:998:ASP:CG	1:A:1001:ARG:HG3	2.36	0.45
1:B:445:TRP:HB3	1:B:579:LEU:HD11	1.97	0.45
1:A:253:ASN:HB2	1:A:286:HIS:HB2	1.99	0.45
1:A:919:ARG:HD2	1:A:1056:LEU:HD23	1.99	0.45
1:B:43:GLY:N	1:B:105:THR:HG21	2.20	0.45
1:B:861:LEU:HD12	1:B:889:PRO:HG3	1.98	0.45
1:B:943:PRO:HD3	1:B:982:SER:O	2.17	0.45
1:B:66:ARG:HH22	1:B:80:LEU:HD11	1.80	0.45
1:B:596:ILE:HG12	1:B:810:LEU:HD11	1.98	0.45
1:A:536:VAL:HA	1:A:546:CYS:HB3	1.97	0.45
1:A:943:PRO:HD3	1:A:982:SER:O	2.17	0.45
1:A:299:GLU:OE2	1:A:301:LYS:HE3	2.17	0.45
1:A:507:PRO:HG2	1:A:508:MET:HG2	1.99	0.45
1:A:648:VAL:HA	1:A:787:GLY:O	2.17	0.45
1:B:487:GLU:HG2	1:B:487:GLU:H	1.55	0.45
1:A:556:PRO:O	1:A:558:THR:N	2.50	0.44
1:B:102:GLY:HA3	1:B:117:TYR:H	1.80	0.44
1:B:448:MET:HB3	1:B:806:MET:HG3	1.97	0.44
1:B:501:PHE:HB2	1:B:544:VAL:HG13	2.00	0.44
1:B:524:GLU:CG	1:B:525:GLU:N	2.81	0.44
1:B:839:ASN:OD1	1:B:845:GLY:HA2	2.17	0.44
1:A:1036:ASN:OD1	1:A:1041:ILE:HG12	2.18	0.44
1:B:154:THR:HG22	1:B:157:MET:CG	2.42	0.44
1:B:569:HIS:C	1:B:571:ASP:H	2.20	0.44
1:A:938:ILE:HG12	1:A:978:LEU:HD23	2.00	0.44
1:B:555:LEU:O	1:B:559:THR:OG1	2.26	0.44
1:A:977:SER:HA	1:A:1010:LYS:HB2	1.99	0.44
1:A:433:HIS:CD2	1:A:585:SER:HB3	2.53	0.44
1:A:574:THR:HB	1:A:575:PRO:HD3	1.98	0.44
1:B:79:VAL:HG11	1:B:108:PRO:HG2	1.98	0.44
1:A:677:SER:OG	1:A:683:VAL:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:HB2	1:A:112:ASP:HB3	2.00	0.44
1:B:840:LYS:HD2	1:B:1034:HIS:CD2	2.52	0.44
1:B:897:ASN:HB3	1:B:1043:ASP:HA	2.00	0.44
1:B:248:ARG:HD2	1:B:248:ARG:HA	1.80	0.44
1:A:250:SER:O	1:A:287:ARG:NH2	2.51	0.43
1:B:556:PRO:O	1:B:558:THR:N	2.51	0.43
1:A:568:ARG:HH11	1:A:571:ASP:HB2	1.83	0.43
1:B:647:ILE:HB	1:B:786:VAL:HG22	2.00	0.43
1:A:859:LEU:HD12	1:A:1012:LYS:HB3	2.00	0.43
1:A:501:PHE:HB2	1:A:544:VAL:HG13	2.00	0.43
1:B:831:ASN:HD22	1:B:1011:HIS:HA	1.83	0.43
1:B:929:ILE:HD13	1:B:960:VAL:CG1	2.48	0.43
1:B:26:LEU:HA	1:B:29:LYS:HD2	2.00	0.43
1:B:299:GLU:OE2	1:B:301:LYS:HE3	2.19	0.43
1:A:3:PRO:O	1:A:4:LEU:C	2.56	0.43
1:B:287:ARG:HG3	1:B:287:ARG:NH1	2.34	0.43
1:B:478:ASN:HB2	1:B:565:ARG:NH1	2.34	0.43
1:B:231:SER:HA	1:B:234:PHE:CD2	2.53	0.43
1:A:159:ILE:HD13	1:A:207:ILE:HG23	2.00	0.43
1:A:523:GLY:HA2	1:A:561:PHE:HA	1.99	0.43
1:B:1000:ARG:NH1	1:B:1000:ARG:HB2	2.33	0.43
1:B:244:ASP:O	1:B:248:ARG:HD3	2.19	0.43
1:B:1004:VAL:O	1:B:1008:ARG:HG2	2.19	0.43
1:B:530:ALA:O	1:B:531:LEU:HB2	2.19	0.43
1:B:84:ARG:HB2	1:B:112:ASP:HB3	2.00	0.43
1:B:880:SER:O	1:B:881:PRO:C	2.57	0.42
1:A:792:LEU:HD12	1:A:972:GLN:OE1	2.19	0.42
1:A:623:ILE:HD13	1:A:664:ARG:HB3	1.99	0.42
1:B:45:ASP:HA	1:B:99:HIS:HE1	1.85	0.42
1:B:471:SER:O	1:B:474:GLU:HG2	2.19	0.42
1:A:198:TYR:O	1:A:754:ARG:HD3	2.18	0.42
1:A:231:SER:HA	1:A:234:PHE:CD2	2.51	0.42
1:A:493:CYS:HB3	1:A:496:GLN:HE21	1.85	0.42
1:B:173:GLU:HB3	1:B:174:SER:H	1.64	0.42
1:B:929:ILE:CD1	1:B:960:VAL:HG11	2.50	0.42
1:A:79:VAL:HG11	1:A:108:PRO:HG2	2.00	0.42
1:B:703:SER:HB3	1:B:714:THR:HG21	2.02	0.42
1:B:839:ASN:OD1	1:B:845:GLY:CA	2.68	0.42
1:A:102:GLY:HA3	1:A:116:GLY:CA	2.48	0.42
1:B:515:ALA:HA	1:B:536:VAL:HB	2.01	0.42
1:B:859:LEU:HD12	1:B:1012:LYS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLU:HB3	1:A:174:SER:H	1.61	0.42
1:A:47:ARG:HG2	1:A:97:ILE:CG2	2.50	0.42
1:A:515:ALA:HA	1:A:536:VAL:HB	2.02	0.42
1:B:104:CYS:O	1:B:105:THR:CB	2.68	0.42
1:A:173:GLU:OE1	1:A:179:ARG:HD3	2.19	0.41
1:A:468:THR:O	1:A:562:ARG:NH2	2.53	0.41
1:A:451:LEU:HB3	1:A:798:ASN:OD1	2.20	0.41
1:A:66:ARG:HH22	1:A:80:LEU:HD11	1.85	0.41
1:B:1038:GLU:HB2	1:B:1040:LEU:HG	2.02	0.41
1:B:192:ARG:NH2	1:B:193:HIS:CE1	2.87	0.41
1:B:55:THR:HA	1:B:64:GLU:O	2.19	0.41
1:A:791:GLN:O	1:A:1000:ARG:HG2	2.20	0.41
1:B:943:PRO:HD2	1:B:984:VAL:HG13	2.02	0.41
1:A:287:ARG:HG3	1:A:287:ARG:NH1	2.35	0.41
1:B:453:SER:HB2	1:B:572:ILE:HG21	2.02	0.41
1:B:507:PRO:HG2	1:B:508:MET:HG2	2.02	0.41
1:B:126:ILE:HD11	1:B:363:ALA:HA	2.02	0.41
1:B:2:GLU:O	1:B:3:PRO:C	2.58	0.41
1:B:40:LEU:HA	1:B:47:ARG:O	2.20	0.41
1:B:102:GLY:HA3	1:B:116:GLY:CA	2.49	0.41
1:A:943:PRO:HD2	1:A:984:VAL:HG13	2.03	0.41
1:A:921:ILE:HD11	1:A:951:ILE:HD13	2.03	0.41
1:A:248:ARG:HA	1:A:248:ARG:HD2	1.78	0.41
1:A:2:GLU:O	1:A:3:PRO:C	2.59	0.41
1:B:790:GLN:O	1:B:1000:ARG:HG3	2.20	0.41
1:B:242:PRO:HD2	1:B:330:GLU:HB3	2.03	0.41
1:B:747:ILE:HG13	1:B:747:ILE:H	1.68	0.41
1:A:318:TYR:HD1	1:A:321:LEU:HD23	1.85	0.41
1:B:521:LEU:HD11	1:B:561:PHE:HB3	2.02	0.41
1:A:1004:VAL:O	1:A:1008:ARG:HG2	2.21	0.41
1:B:223:GLU:O	1:B:227:ARG:HB3	2.21	0.41
1:A:829:ARG:NE	1:A:975:ASP:HB3	2.36	0.41
1:A:929:ILE:HD13	1:A:960:VAL:HG11	2.03	0.41
1:A:608:LEU:HD21	1:B:178:GLU:HB3	2.03	0.41
1:B:183:LEU:O	1:B:187:THR:CG2	2.60	0.41
1:B:921:ILE:HD11	1:B:951:ILE:HD13	2.02	0.40
1:A:104:CYS:O	1:A:105:THR:CB	2.69	0.40
1:A:140:ARG:HG3	1:A:397:CYS:SG	2.61	0.40
1:A:760:CYS:SG	1:A:776:PRO:HB2	2.61	0.40
1:A:102:GLY:HA3	1:A:117:TYR:H	1.83	0.40
1:B:159:ILE:HD12	1:B:210:GLU:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:PRO:O	1:B:4:LEU:C	2.59	0.40
1:A:2:GLU:N	1:A:6:GLU:HG3	2.36	0.40
1:A:374:ALA:HA	1:A:375:PRO:HD2	1.96	0.40
1:A:480:VAL:HG23	1:A:513:LEU:HD22	2.02	0.40
1:B:654:GLY:HA2	3:B:1102:ADP:O2B	2.21	0.40
1:B:199:ARG:HG3	1:B:753:SER:OG	2.21	0.40
1:B:759:PHE:HA	1:B:782:ARG:O	2.22	0.40
1:A:126:ILE:HG21	1:A:362:LEU:HD23	2.04	0.40
1:A:596:ILE:HG12	1:A:810:LEU:HD11	2.02	0.40
1:B:140:ARG:HG3	1:B:397:CYS:SG	2.62	0.40
1:B:387:ILE:HG23	2:B:1101:SF4:S3	2.61	0.40
1:B:493:CYS:HB3	1:B:496:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1038/1056 (98%)	916 (88%)	90 (9%)	32 (3%)	4 23
1	B	1038/1056 (98%)	919 (88%)	85 (8%)	34 (3%)	4 21
All	All	2076/2112 (98%)	1835 (88%)	175 (8%)	66 (3%)	4 22

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	105	THR
1	A	375	PRO
1	A	508	MET
1	A	524	GLU
1	A	874	TYR

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Mol	Chain	Res	Type
1	A	989	ASP
1	B	2	GLU
1	B	105	THR
1	B	375	PRO
1	B	508	MET
1	B	524	GLU
1	B	554	THR
1	B	565	ARG
1	B	566	GLU
1	B	567	GLU
1	B	874	TYR
1	B	989	ASP
1	A	4	LEU
1	A	554	THR
1	A	557	ALA
1	A	565	ARG
1	A	569	HIS
1	A	959	SER
1	B	4	LEU
1	B	417	ALA
1	B	530	ALA
1	B	557	ALA
1	B	569	HIS
1	B	959	SER
1	A	109	TRP
1	A	417	ALA
1	A	530	ALA
1	A	531	LEU
1	B	109	TRP
1	B	723	SER
1	B	984	VAL
1	A	40	LEU
1	A	244	ASP
1	A	492	VAL
1	A	511	THR
1	A	984	VAL
1	B	40	LEU
1	B	492	VAL
1	B	494	ASP
1	B	531	LEU
1	A	250	SER
1	A	416	ASP

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Mol	Chain	Res	Type
1	A	494	ASP
1	A	507	PRO
1	A	723	SER
1	A	881	PRO
1	B	244	ASP
1	B	250	SER
1	B	416	ASP
1	B	507	PRO
1	B	511	THR
1	B	515	ALA
1	B	881	PRO
1	B	75	ARG
1	A	509	PRO
1	A	481	GLY
1	B	509	PRO
1	A	3	PRO
1	A	385	PRO
1	B	481	GLY

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	931/937 (99%)	845 (91%)	86 (9%)	9 34
1	B	931/937 (99%)	844 (91%)	87 (9%)	9 33
All	All	1862/1874 (99%)	1689 (91%)	173 (9%)	9 33

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	47	ARG
1	A	54	GLU
1	A	57	GLN
1	A	74	ASP

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Mol	Chain	Res	Type
1	A	93	GLU
1	A	100	LEU
1	A	101	GLU
1	A	136	ARG
1	A	140	ARG
1	A	144	SER
1	A	150	SER
1	A	174	SER
1	A	183	LEU
1	A	185	LEU
1	A	186	GLN
1	A	187	THR
1	A	191	VAL
1	A	208	LEU
1	A	233	GLU
1	A	248	ARG
1	A	287	ARG
1	A	304	LYS
1	A	321	LEU
1	A	354	GLU
1	A	359	ARG
1	A	370	VAL
1	A	372	ARG
1	A	378	GLU
1	A	386	GLN
1	A	389	GLU
1	A	391	GLU
1	A	400	ILE
1	A	410	VAL
1	A	424	LEU
1	A	456	LYS
1	A	457	ASP
1	A	458	ASN
1	A	460	LYS
1	A	486	THR
1	A	491	ARG
1	A	502	GLN
1	A	504	LYS
1	A	505	ASN
1	A	511	THR
1	A	512	ASN
1	A	513	LEU

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Mol	Chain	Res	Type
1	A	526	ARG
1	A	538	LYS
1	A	546	CYS
1	A	547	LEU
1	A	558	THR
1	A	559	THR
1	A	562	ARG
1	A	568	ARG
1	A	601	GLU
1	A	609	SER
1	A	612	LEU
1	A	615	ASP
1	A	673	VAL
1	A	681	SER
1	A	716	GLU
1	A	751	ILE
1	A	781	ARG
1	A	819	SER
1	A	838	SER
1	A	859	LEU
1	A	864	LEU
1	A	868	ARG
1	A	874	TYR
1	A	896	LEU
1	A	906	GLN
1	A	913	SER
1	A	916	THR
1	A	926	SER
1	A	946	GLN
1	A	962	MET
1	A	963	VAL
1	A	980	LEU
1	A	984	VAL
1	A	987	ASN
1	A	1000	ARG
1	A	1018	SER
1	A	1041	ILE
1	A	1043	ASP
1	A	1047	ARG
1	B	1	MET
1	B	47	ARG
1	B	54	GLU

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Mol	Chain	Res	Type
1	B	57	GLN
1	B	74	ASP
1	B	100	LEU
1	B	101	GLU
1	B	136	ARG
1	B	140	ARG
1	B	150	SER
1	B	183	LEU
1	B	185	LEU
1	B	186	GLN
1	B	187	THR
1	B	191	VAL
1	B	208	LEU
1	B	233	GLU
1	B	248	ARG
1	B	287	ARG
1	B	304	LYS
1	B	321	LEU
1	B	335	LEU
1	B	354	GLU
1	B	359	ARG
1	B	370	VAL
1	B	372	ARG
1	B	378	GLU
1	B	389	GLU
1	B	391	GLU
1	B	400	ILE
1	B	405	LEU
1	B	410	VAL
1	B	424	LEU
1	B	456	LYS
1	B	457	ASP
1	B	458	ASN
1	B	460	LYS
1	B	486	THR
1	B	487	GLU
1	B	491	ARG
1	B	502	GLN
1	B	504	LYS
1	B	505	ASN
1	B	511	THR
1	B	512	ASN

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Mol	Chain	Res	Type
1	B	513	LEU
1	B	526	ARG
1	B	538	LYS
1	B	546	CYS
1	B	547	LEU
1	B	558	THR
1	B	559	THR
1	B	562	ARG
1	B	568	ARG
1	B	601	GLU
1	B	612	LEU
1	B	615	ASP
1	B	673	VAL
1	B	681	SER
1	B	716	GLU
1	B	751	ILE
1	B	781	ARG
1	B	819	SER
1	B	838	SER
1	B	859	LEU
1	B	868	ARG
1	B	874	TYR
1	B	896	LEU
1	B	906	GLN
1	B	916	THR
1	B	926	SER
1	B	933	CYS
1	B	946	GLN
1	B	962	MET
1	B	963	VAL
1	B	969	ASP
1	B	980	LEU
1	B	984	VAL
1	B	987	ASN
1	B	991	THR
1	B	996	LEU
1	B	1000	ARG
1	B	1018	SER
1	B	1028	LEU
1	B	1041	ILE
1	B	1043	ASP
1	B	1047	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	314	GLN
1	A	323	GLN
1	A	458	ASN
1	A	496	GLN
1	A	505	ASN
1	A	770	GLN
1	A	946	GLN
1	A	972	GLN
1	A	1034	HIS
1	B	164	HIS
1	B	314	GLN
1	B	458	ASN
1	B	496	GLN
1	B	505	ASN
1	B	946	GLN
1	B	1034	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	A	1102	-	24,29,29	1.16	3 (12%)	29,45,45	1.42	4 (13%)
2	SF4	A	1101	1	0,12,12	0.00	-	-		
2	SF4	B	1101	1	0,12,12	0.00	-	-		
3	ADP	B	1102	-	24,29,29	1.15	2 (8%)	29,45,45	1.46	4 (13%)

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	ADP	A	1102	-	-	6/12/32/32	0/3/3/3
2	SF4	A	1101	1	-	-	0/6/5/5
2	SF4	B	1101	1	-	-	0/6/5/5
3	ADP	B	1102	-	-	6/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	ADP	C5-C4	2.91	1.48	1.40
3	A	1102	ADP	C5-C4	2.88	1.48	1.40
3	B	1102	ADP	C2-N3	2.51	1.36	1.32
3	A	1102	ADP	O4'-C1'	2.23	1.44	1.41
3	A	1102	ADP	C2-N3	2.00	1.35	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1102	ADP	N3-C2-N1	-3.47	123.25	128.68
3	B	1102	ADP	C3'-C2'-C1'	3.18	105.77	100.98
3	B	1102	ADP	N3-C2-N1	-3.15	123.75	128.68
3	A	1102	ADP	C4-C5-N7	-2.93	106.34	109.40
3	B	1102	ADP	PA-O3A-PB	-2.86	123.02	132.83
3	B	1102	ADP	C4-C5-N7	-2.68	106.61	109.40
3	A	1102	ADP	C3'-C2'-C1'	2.46	104.68	100.98
3	A	1102	ADP	PA-O3A-PB	-2.21	125.24	132.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	ADP	PA-O3A-PB-O2B
3	B	1102	ADP	PA-O3A-PB-O2B
3	A	1102	ADP	O4'-C4'-C5'-O5'
3	B	1102	ADP	O4'-C4'-C5'-O5'
3	A	1102	ADP	C3'-C4'-C5'-O5'
3	B	1102	ADP	C3'-C4'-C5'-O5'
3	B	1102	ADP	C4'-C5'-O5'-PA
3	A	1102	ADP	C4'-C5'-O5'-PA
3	A	1102	ADP	PA-O3A-PB-O1B
3	B	1102	ADP	PA-O3A-PB-O1B
3	A	1102	ADP	C5'-O5'-PA-O1A
3	B	1102	ADP	C5'-O5'-PA-O1A

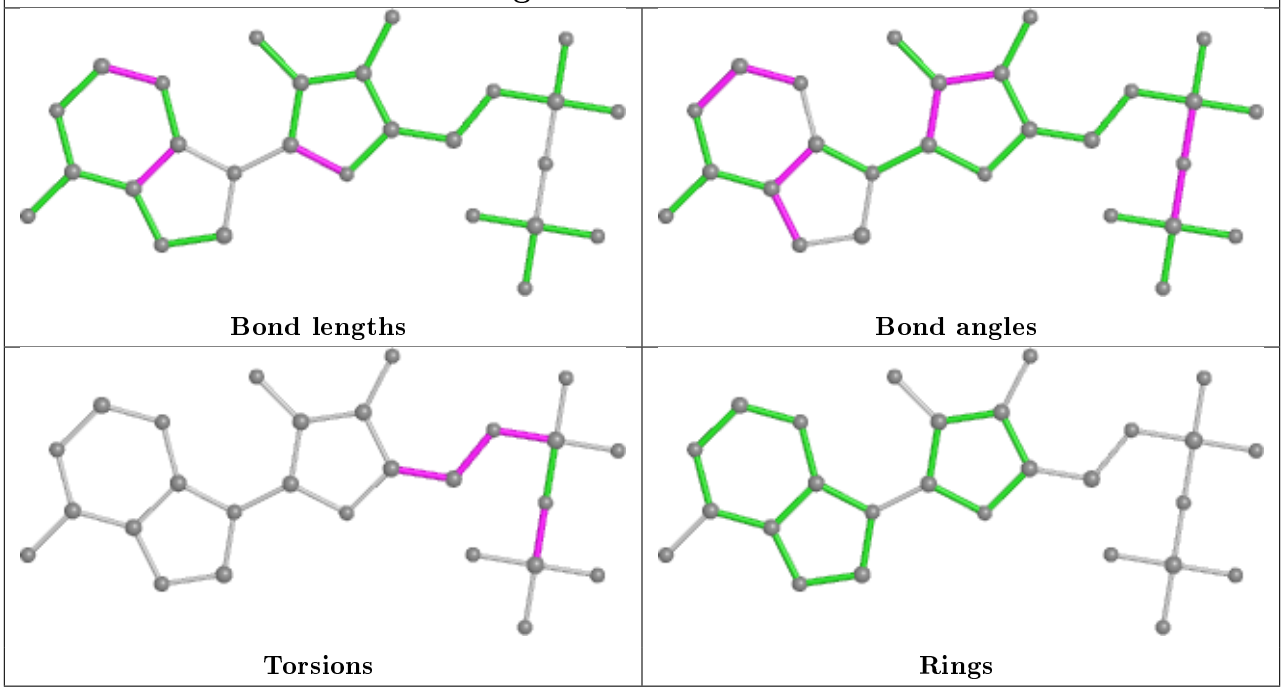
There are no ring outliers.

3 monomers are involved in 3 short contacts:

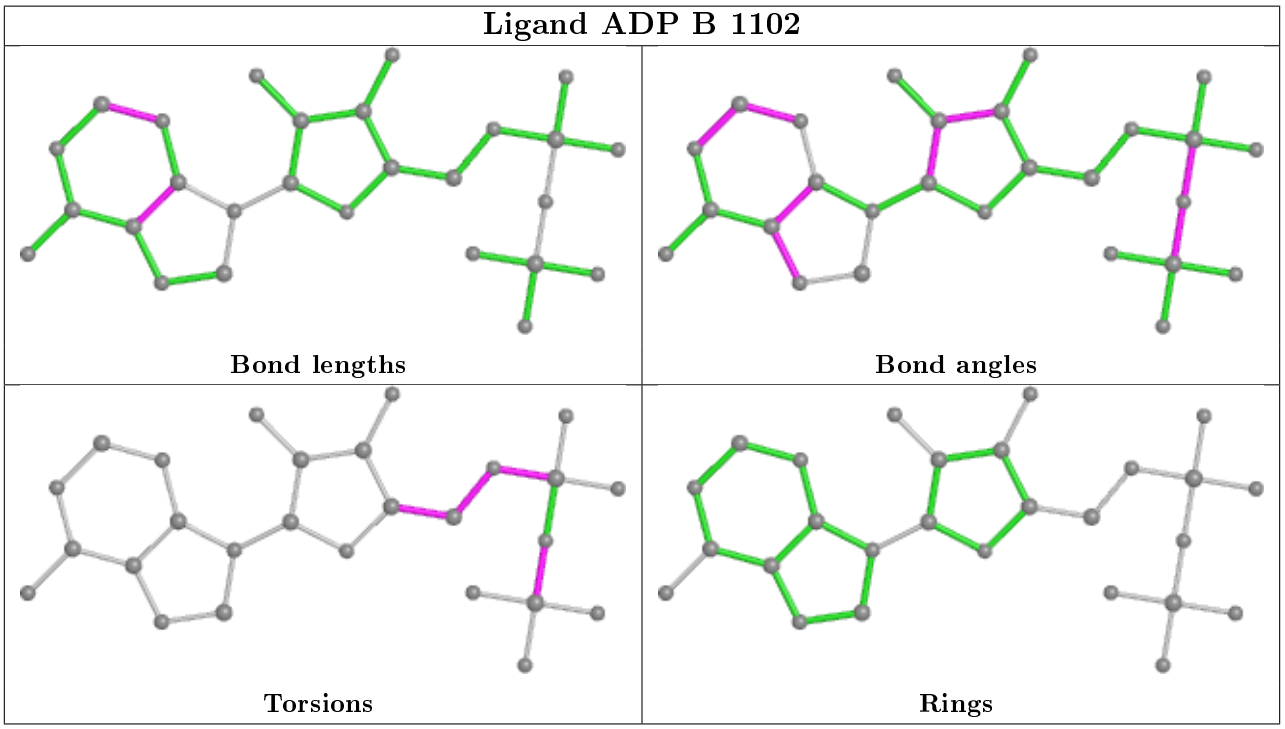
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	ADP	1	0
2	B	1101	SF4	1	0
3	B	1102	ADP	1	0

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 then 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 ADP A 1102



Ligand ADP B 1102



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	1046/1056 (99%)	-0.38	9 (0%)	84	63	24, 53, 119, 169	0
1	B	1046/1056 (99%)	-0.34	10 (0%)	82	59	23, 56, 126, 193	0
All	All	2092/2112 (99%)	-0.36	19 (0%)	84	63	23, 55, 123, 193	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	ASP	4.7
1	B	103	ASP	4.2
1	B	106	SER	3.6
1	B	478	ASN	3.3
1	B	877	TYR	2.9
1	A	507	PRO	2.8
1	B	375	PRO	2.7
1	A	245	GLY	2.4
1	A	248	ARG	2.4
1	B	880	SER	2.3
1	A	884	ALA	2.3
1	B	505	ASN	2.2
1	A	505	ASN	2.2
1	B	879	ASP	2.2
1	A	415	ASP	2.2
1	B	871	LEU	2.2
1	A	103	ASP	2.2
1	A	879	ASP	2.1
1	A	244	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

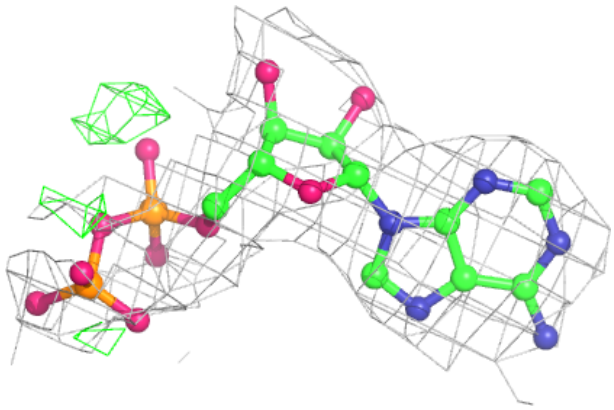
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

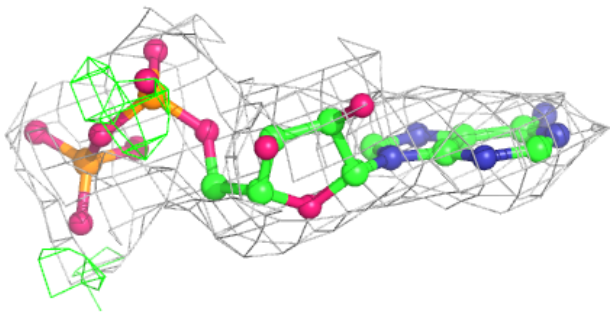
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	A	1102	27/27	0.85	0.19	63,86,136,141	0
3	ADP	B	1102	27/27	0.86	0.20	62,99,131,140	0
2	SF4	B	1101	8/8	0.99	0.11	57,63,71,72	0
2	SF4	A	1101	8/8	0.99	0.10	51,58,63,64	0

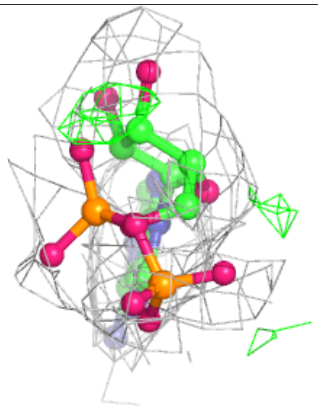
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1102:

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

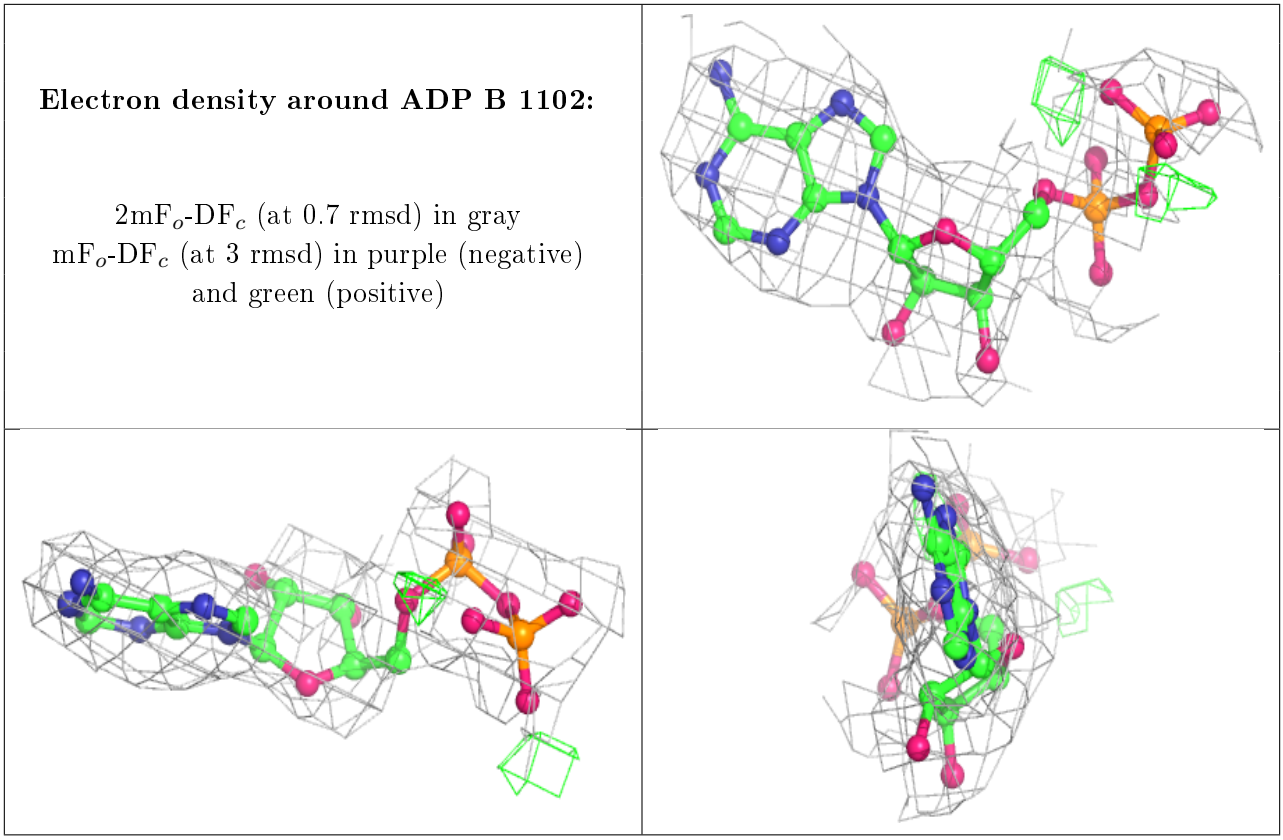






Electron density around ADP B 1102:

$2mF_o$-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

There are no such residues in this entry.