Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:30 PM GMT

PDB ID	:	4CEJ
Title	:	Crystal structure of ADPNP-bound AddAB bound to Chi
Authors	:	Krajewski, W.W.; Wilkinson, M.; Fu, X.; Cronin, N.B.; Wigley, D.
Deposited on	:	2013-11-11
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

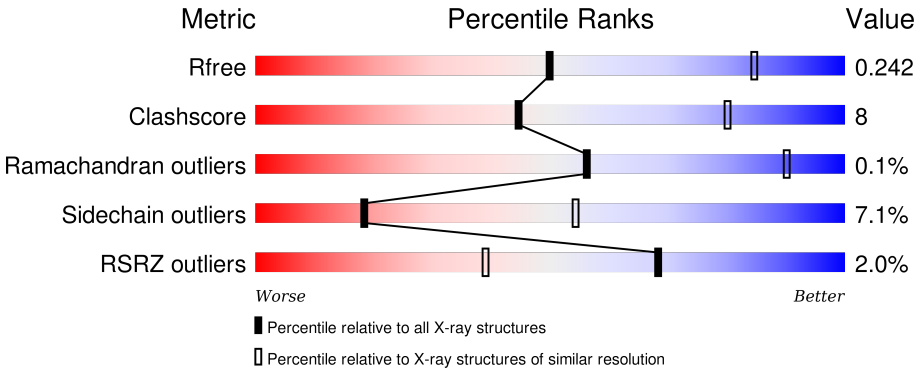
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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. 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	1232	3% 71% 22%
2	B	1166	% 77% 21%
3	X	70	6% 44% 20% 34%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19953 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 ATP-DEPENDENT HELICASE/NUCLEASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1177	Total	C	N	O	S	0	0	0
			9539	6084	1627	1800	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	780	GLY	ALA	VARIANT	UNP P23478
A	1172	ALA	ASP	ENGINEERED MUTATION	UNP P23478

- Molecule 2 is a protein called ATP-DEPENDENT HELICASE/DEOXYRIBONUCLEASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1156	Total	C	N	O	S	0	1	0
			9410	5979	1613	1774	44			

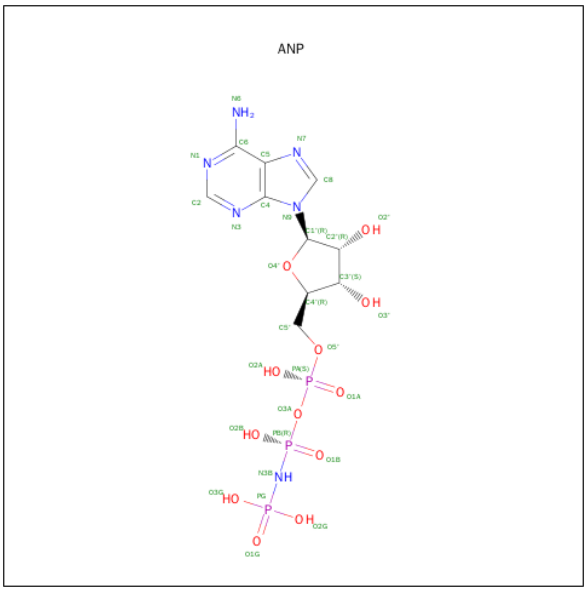
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	843	ASP	GLU	VARIANT	UNP P23477
B	844	GLU	GLN	VARIANT	UNP P23477
B	961	ALA	ASP	ENGINEERED MUTATION	UNP P23477

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	46	Total	C	N	O	P	0	0	0
			925	443	151	285	46			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

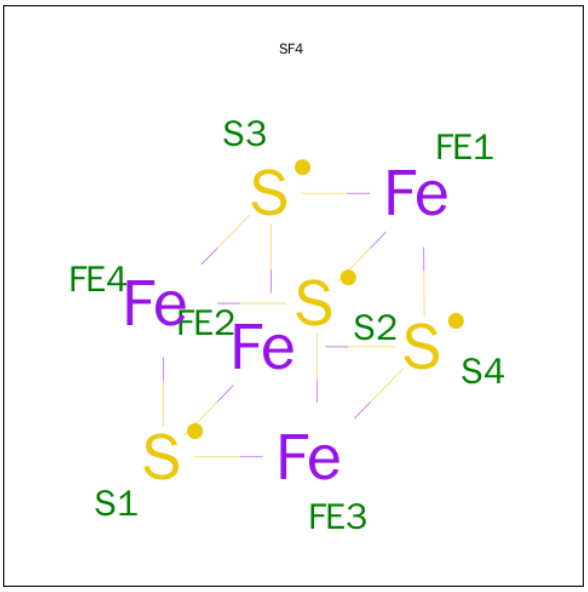


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 7 is water.

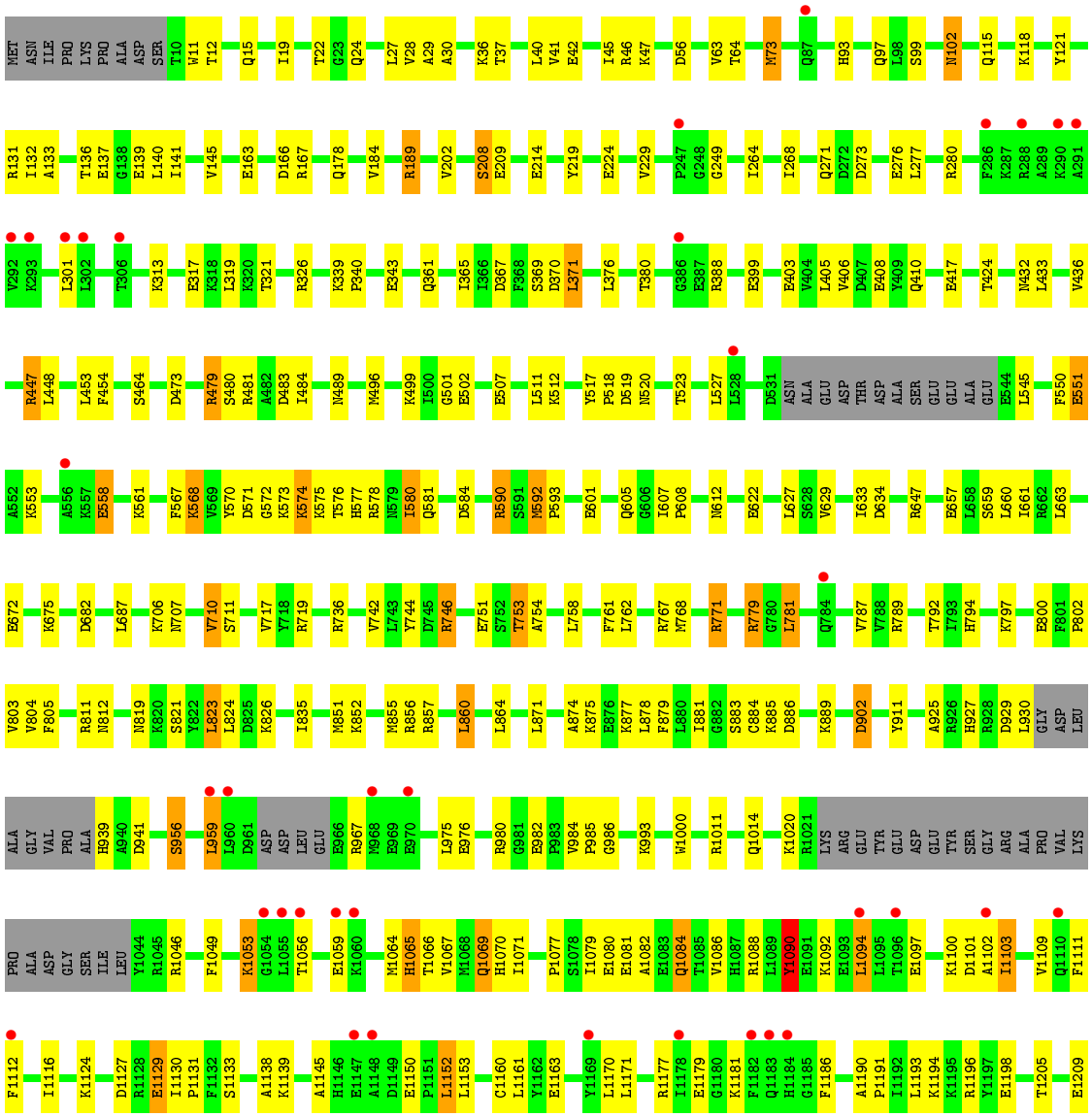
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	4	Total O 4 4	0	0
7	B	3	Total O 3 3	0	0

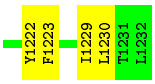
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ATP-DEPENDENT HELICASE/NUCLEASE SUBUNIT A

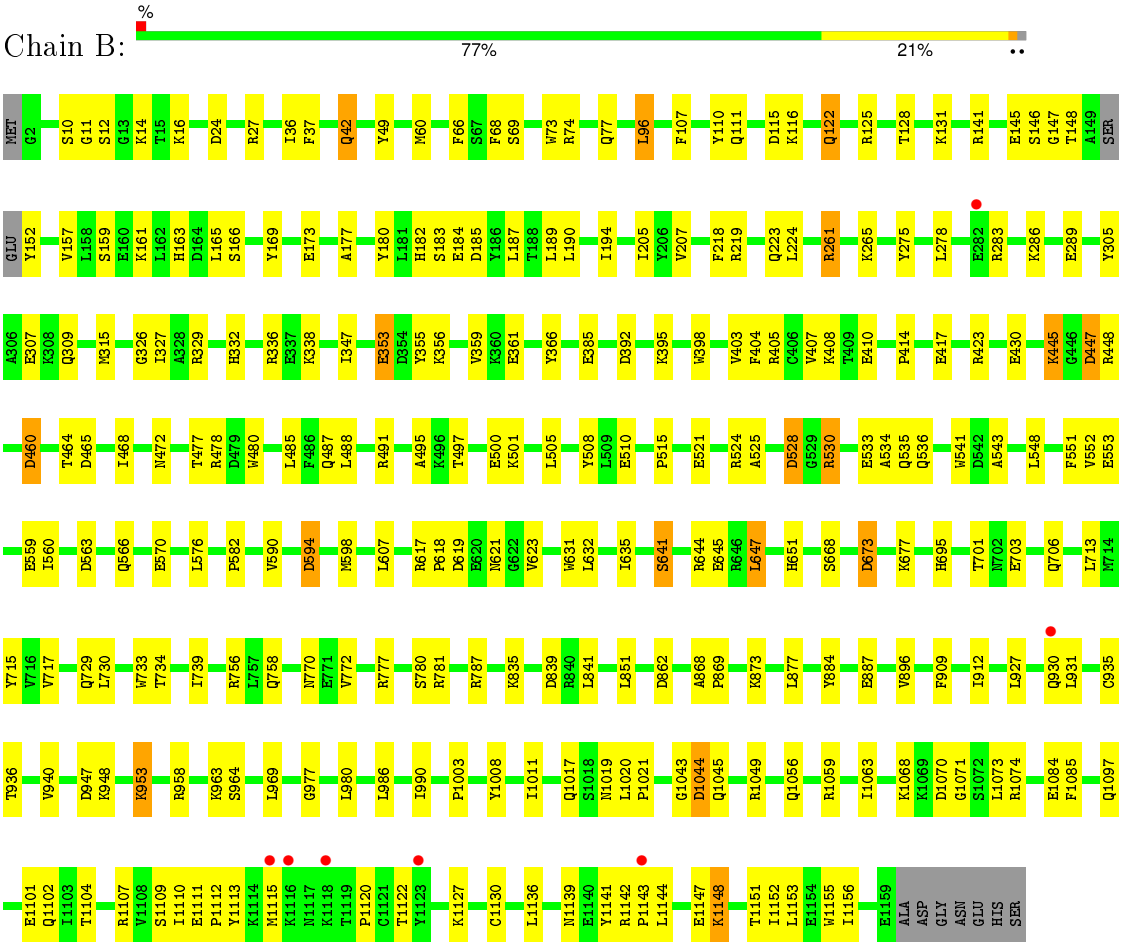
Chain A:





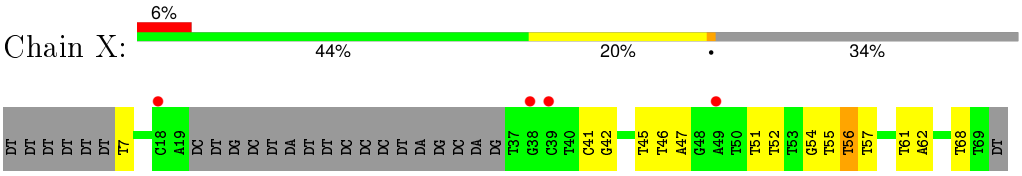
• Molecule 2: ATP-DEPENDENT HELICASE/DEOXYRIBONUCLEASE SUBUNIT B

Chain B:



• Molecule 3: DNA

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.44Å 152.94Å 125.24Å 90.00° 94.30° 90.00°	Depositor
Resolution (Å)	29.73 – 3.00 35.55 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.73-3.00) 99.7 (35.55-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 3.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.203 , 0.243 0.204 , 0.242	Depositor DCC
R_{free} test set	2921 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	71.6	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 62.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 57977 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19953	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0.25	0/9731	0.44	2/13128 (0.0%)
2	B	0.24	0/9601	0.42	0/12936
3	X	0.66	0/1031	1.15	1/1589 (0.1%)
All	All	0.28	0/20363	0.50	3/27653 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	56	DT	O4'-C1'-N1	6.68	112.68	108.00
1	A	1090	TYR	CA-CB-CG	5.15	123.18	113.40
1	A	986	GLY	N-CA-C	5.03	125.67	113.10

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	9539	0	9505	182	0
2	B	9410	0	9357	136	0
3	X	925	0	516	16	0
4	A	31	0	13	2	0
4	B	31	0	13	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	8	0	0	1	0
7	A	4	0	0	0	0
7	B	3	0	0	0	0
All	All	19953	0	19404	309	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 8.

All (309) 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)
2:B:912:ILE:HD11	2:B:948:LYS:HB3	1.64	0.79
2:B:165:LEU:HD11	2:B:623:VAL:HG11	1.65	0.77
1:A:30:ALA:HB3	1:A:36:LYS:HD2	1.68	0.75
2:B:414:PRO:HB2	2:B:417:GLU:HG3	1.68	0.74
1:A:28:VAL:HB	1:A:436:VAL:HG12	1.69	0.74
1:A:276:GLU:HG3	1:A:280:ARG:HE	1.52	0.72
1:A:167:ARG:NH1	1:A:835:ILE:O	2.22	0.72
1:A:590:ARG:HH21	1:A:794:HIS:HE1	1.37	0.70
1:A:856:ARG:NH1	1:A:911:TYR:O	2.25	0.69
1:A:417:GLU:HB2	1:A:453:LEU:HD21	1.74	0.69
1:A:578:ARG:NH2	1:A:584:ASP:OD1	2.26	0.69
1:A:479:ARG:HD3	1:A:800:GLU:HB3	1.75	0.69
1:A:480:SER:OG	1:A:874:ALA:O	2.10	0.68
2:B:180:TYR:OH	2:B:553:GLU:OE1	2.13	0.67
1:A:166:ASP:OD1	2:B:884:TYR:OH	2.11	0.67
2:B:11:GLY:H	4:B:2161:ANP:HNB1	1.42	0.67
2:B:1115:MET:HB2	2:B:1144:LEU:HB2	1.75	0.67
2:B:703:GLU:OE1	2:B:706:GLN:NE2	2.27	0.67
2:B:896:VAL:HG21	2:B:1011:ILE:HG23	1.79	0.65
2:B:930:GLN:O	2:B:1097:GLN:NE2	2.30	0.65
2:B:772:VAL:HG21	2:B:1109:SER:HA	1.79	0.65
2:B:835:LYS:NZ	2:B:839:ASP:OD2	2.30	0.65
2:B:787:ARG:HG3	2:B:787:ARG:HH11	1.63	0.64
1:A:578:ARG:NH1	1:A:581:GLN:OE1	2.31	0.64
2:B:448:ARG:HH22	2:B:472:ASN:HA	1.63	0.64
1:A:1077:PRO:HD2	1:A:1112:PHE:HD2	1.63	0.64
2:B:1111:GLU:HB3	2:B:1142:ARG:HD3	1.80	0.64
2:B:521:GLU:OE2	2:B:524:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:ARG:HH21	2:B:772:VAL:HG12	1.62	0.62
2:B:283:ARG:HD3	4:B:2161:ANP:H4'	1.80	0.62
2:B:488:LEU:HD13	2:B:508:TYR:HB2	1.82	0.62
1:A:1138:ALA:HA	1:A:1152:LEU:HD11	1.81	0.62
2:B:385:GLU:OE2	2:B:405:ARG:NH1	2.33	0.62
1:A:1079:ILE:HA	1:A:1109:VAL:HG21	1.80	0.61
2:B:931:LEU:HD12	2:B:935:CYS:HB2	1.81	0.61
2:B:460:ASP:N	2:B:460:ASP:OD1	2.33	0.61
1:A:380:THR:HG21	1:A:388:ARG:HE	1.65	0.61
2:B:1113:TYR:CE2	2:B:1120:PRO:HG3	2.36	0.61
1:A:819:ASN:HB3	3:X:7:DT:H4'	1.81	0.61
1:A:131:ARG:NH2	1:A:137:GLU:OE2	2.33	0.60
1:A:871:LEU:HD22	1:A:878:LEU:HD21	1.83	0.60
1:A:812:ASN:HB2	3:X:51:DT:H5"	1.83	0.60
2:B:528:ASP:HB3	2:B:530:ARG:HD3	1.84	0.60
2:B:447:ASP:N	2:B:447:ASP:OD1	2.32	0.59
2:B:10:SER:OG	2:B:283:ARG:NH2	2.35	0.59
1:A:313:LYS:NZ	3:X:42:DG:OP2	2.36	0.59
1:A:571:ASP:O	1:A:575:LYS:N	2.34	0.59
2:B:305:TYR:CZ	2:B:307:GLU:HB2	2.37	0.59
2:B:947:ASP:HB2	2:B:958:ARG:HG2	1.85	0.58
1:A:1082:ALA:O	1:A:1086:VAL:HG23	2.03	0.58
1:A:1011:ARG:HD3	2:B:582:PRO:HB2	1.85	0.58
1:A:481:ARG:NH2	1:A:518:PRO:O	2.36	0.58
1:A:612:ASN:HD22	1:A:779:ARG:HD2	1.68	0.58
1:A:811:ARG:NH2	3:X:52:DT:OP1	2.37	0.57
2:B:594:ASP:N	2:B:594:ASP:OD1	2.37	0.57
1:A:1111:PHE:HB2	1:A:1222:TYR:CZ	2.40	0.57
1:A:802:PRO:HA	1:A:875:LYS:HB2	1.87	0.57
1:A:121:TYR:OH	2:B:122:GLN:NE2	2.38	0.56
1:A:711:SER:N	1:A:751:GLU:OE2	2.36	0.56
1:A:1133:SER:HB3	1:A:1153:LEU:HD11	1.86	0.56
1:A:321:THR:O	2:B:1019:ASN:ND2	2.38	0.56
2:B:909:PHE:HB3	2:B:947:ASP:HB3	1.88	0.56
1:A:1124:LYS:NZ	1:A:1163:GLU:OE1	2.35	0.56
2:B:1059:ARG:HD3	3:X:45:DT:H5"	1.88	0.56
1:A:805:PHE:HD2	1:A:881:ILE:HD11	1.71	0.56
3:X:68:DT:H5'	3:X:68:DT:C6	2.40	0.55
1:A:141:ILE:HD12	1:A:365:ILE:HD11	1.87	0.55
1:A:408:GLU:OE1	1:A:410:GLN:NE2	2.31	0.55
2:B:205:ILE:HD13	2:B:224:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:787:ARG:NH1	2:B:936:THR:OG1	2.40	0.55
1:A:984:VAL:HG13	1:A:985:PRO:HD2	1.88	0.55
3:X:55:DT:H2"	3:X:56:DT:O5'	2.08	0.54
2:B:977:GLY:HA2	2:B:980:LEU:HD21	1.89	0.54
2:B:963:LYS:HG3	2:B:1008:TYR:HD2	1.72	0.54
2:B:14:LYS:NZ	4:B:2161:ANP:O2B	2.27	0.53
2:B:131:LYS:NZ	2:B:173:GLU:OE2	2.35	0.53
2:B:990:ILE:HG13	2:B:1003:PRO:HG3	1.90	0.53
2:B:953:LYS:NZ	2:B:1044:ASP:OD1	2.39	0.53
2:B:329:ARG:HD3	2:B:715:TYR:HA	1.90	0.53
2:B:16:LYS:HD3	4:B:2161:ANP:C8	2.39	0.53
2:B:157:VAL:HG12	2:B:161:LYS:HE3	1.91	0.53
2:B:1112:PRO:HG3	6:B:2160:SF4:S4	2.49	0.53
2:B:12:SER:HB3	2:B:278:LEU:HB2	1.90	0.52
2:B:125:ARG:HG2	3:X:61:DT:H72	1.91	0.52
2:B:770:ASN:H	2:B:1136:LEU:HD21	1.72	0.52
1:A:141:ILE:O	1:A:145:VAL:HG13	2.10	0.52
1:A:11:TRP:HZ2	1:A:42:GLU:HG3	1.74	0.52
1:A:133:ALA:HB2	1:A:365:ILE:HD12	1.92	0.52
1:A:567:PHE:HB3	1:A:580:ILE:HG13	1.92	0.52
1:A:1194:LYS:NZ	1:A:1198:GLU:OE2	2.39	0.51
2:B:141:ARG:O	2:B:145:GLU:HG2	2.10	0.51
1:A:622:GLU:HG2	1:A:736:ARG:HB3	1.92	0.51
1:A:264:ILE:O	1:A:268:ILE:HG13	2.11	0.51
1:A:975:LEU:HG	2:B:733:TRP:HZ3	1.75	0.51
1:A:975:LEU:HG	2:B:733:TRP:CZ3	2.45	0.51
2:B:501:LYS:NZ	2:B:560:ILE:O	2.36	0.51
2:B:16:LYS:HD3	4:B:2161:ANP:N7	2.26	0.51
1:A:229:VAL:HG21	1:A:319:LEU:HD13	1.92	0.51
2:B:392:ASP:OD2	2:B:405:ARG:NH2	2.43	0.51
1:A:1097:GLU:HG2	1:A:1100:LYS:HD2	1.92	0.51
1:A:1090:TYR:CD1	1:A:1090:TYR:C	2.83	0.51
1:A:1116:ILE:HD12	1:A:1229:ILE:HG21	1.93	0.51
1:A:1160:CYS:HB3	1:A:1171:LEU:HB3	1.93	0.51
2:B:289:GLU:OE1	2:B:695:HIS:NE2	2.34	0.51
1:A:574:LYS:O	1:A:574:LYS:HD2	2.11	0.51
2:B:410:GLU:OE2	2:B:423:ARG:NH1	2.37	0.51
1:A:1127:ASP:HB3	1:A:1130:ILE:HD11	1.94	0.50
2:B:969:LEU:HB2	2:B:1008:TYR:HE1	1.76	0.50
1:A:479:ARG:NH2	4:A:2233:ANP:HNB1	2.09	0.50
1:A:612:ASN:HD22	1:A:779:ARG:HH11	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:THR:HG22	1:A:754:ALA:N	2.25	0.50
1:A:902:ASP:OD1	1:A:902:ASP:N	2.42	0.50
1:A:1069:GLN:HA	1:A:1069:GLN:HE21	1.76	0.50
1:A:273:ASP:OD2	1:A:276:GLU:HB2	2.12	0.50
1:A:884:CYS:SG	1:A:885:LYS:N	2.85	0.49
1:A:605:GLN:HB2	1:A:607:ILE:HD12	1.94	0.49
2:B:347:ILE:HG23	2:B:607:LEU:HD13	1.94	0.49
2:B:1102:GLN:OE1	2:B:1107:ARG:NH1	2.42	0.49
1:A:925:ALA:HA	1:A:930:LEU:HD23	1.94	0.49
1:A:823:LEU:HD21	1:A:855:MET:SD	2.53	0.49
1:A:1205:THR:O	1:A:1209:GLU:HB2	2.13	0.49
2:B:1147:GLU:HG3	2:B:1155:TRP:CH2	2.48	0.49
1:A:479:ARG:HH22	4:A:2233:ANP:HNB1	1.60	0.49
2:B:326:GLY:HA2	2:B:329:ARG:NH1	2.27	0.49
2:B:42:GLN:H	2:B:42:GLN:CD	2.16	0.49
1:A:403:GLU:HA	1:A:432:ASN:HB2	1.94	0.49
1:A:11:TRP:CZ2	1:A:42:GLU:HG3	2.48	0.49
2:B:366:TYR:CD2	2:B:717:VAL:HG21	2.47	0.48
2:B:543:ALA:HB1	2:B:576:LEU:HD22	1.95	0.48
1:A:64:THR:HG22	1:A:73:MET:HE1	1.95	0.48
2:B:36:ILE:HG23	2:B:66:PHE:HD2	1.78	0.48
1:A:792:THR:OG1	3:X:54:DG:OP1	2.18	0.48
1:A:742:VAL:O	1:A:746:ARG:HD3	2.13	0.48
2:B:1068:LYS:HB2	2:B:1070:ASP:OD1	2.14	0.48
1:A:27:LEU:HD11	1:A:454:PHE:CE2	2.48	0.48
2:B:1153:LEU:HA	2:B:1156:ILE:HD12	1.94	0.48
2:B:404:PHE:CZ	2:B:430:GLU:HA	2.49	0.48
2:B:1148:LYS:O	2:B:1151:THR:OG1	2.19	0.48
2:B:730:LEU:O	2:B:734:THR:HG23	2.14	0.48
1:A:980:ARG:NH1	1:A:982:GLU:OE2	2.46	0.48
2:B:110:TYR:OH	2:B:623:VAL:HG13	2.14	0.47
1:A:132:ILE:N	3:X:57:DT:O4	2.25	0.47
2:B:355:TYR:O	2:B:359:VAL:HG23	2.15	0.47
1:A:184:VAL:HG22	1:A:824:LEU:HD21	1.97	0.47
1:A:1102:ALA:O	1:A:1103:ILE:HG12	2.15	0.47
2:B:261[B]:ARG:HG2	2:B:261[B]:ARG:HH11	1.80	0.47
1:A:507:GLU:O	1:A:512:LYS:NZ	2.38	0.47
1:A:523:THR:HA	1:A:877:LYS:HD3	1.96	0.47
2:B:477:THR:HA	2:B:480:TRP:NE1	2.30	0.47
1:A:823:LEU:HB3	1:A:851:MET:HE1	1.96	0.47
1:A:1064:MET:SD	1:A:1103:ILE:HD13	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:LYS:HD3	2:B:566:GLN:OE1	2.14	0.47
2:B:182:HIS:HB3	2:B:185:ASP:OD2	2.15	0.47
2:B:403:VAL:O	2:B:407:VAL:HG23	2.14	0.47
1:A:570:TYR:HD1	1:A:577:HIS:CE1	2.32	0.47
2:B:115:ASP:HB3	2:B:116:LYS:HZ2	1.80	0.47
1:A:214:GLU:HA	1:A:219:TYR:CD2	2.49	0.47
1:A:657:GLU:HB3	1:A:687:LEU:HD13	1.97	0.47
2:B:147:GLY:HA3	2:B:159:SER:HB3	1.96	0.47
1:A:993:LYS:HD2	2:B:713:LEU:HD21	1.96	0.47
2:B:42:GLN:OE1	3:X:62:DA:H1'	2.13	0.46
2:B:353:GLU:OE1	2:B:356:LYS:NZ	2.37	0.46
1:A:1071:ILE:HG21	1:A:1112:PHE:HZ	1.79	0.46
1:A:781:LEU:HD22	1:A:787:VAL:HG11	1.96	0.46
2:B:1141:TYR:O	2:B:1143:PRO:HD3	2.16	0.46
1:A:484:ILE:HD12	1:A:878:LEU:HB2	1.98	0.46
2:B:96:LEU:HA	2:B:96:LEU:HD12	1.79	0.46
1:A:371:LEU:HA	1:A:371:LEU:HD12	1.81	0.46
1:A:1161:LEU:HD23	1:A:1170:LEU:HA	1.96	0.46
1:A:629:VAL:O	1:A:633:ILE:HG13	2.16	0.46
1:A:367:ASP:HB3	1:A:369:SER:H	1.80	0.46
1:A:719:ARG:NH2	2:B:361:GLU:OE1	2.48	0.46
2:B:641:SER:OG	2:B:645:GLU:OE1	2.28	0.46
1:A:551:GLU:OE1	1:A:883:SER:OG	2.25	0.46
1:A:1020:LYS:NZ	1:A:1196:ARG:O	2.39	0.46
1:A:1139:LYS:HD3	1:A:1145:ALA:O	2.16	0.46
1:A:224:GLU:OE1	1:A:857:ARG:NH1	2.49	0.45
1:A:976:GLU:O	1:A:980:ARG:HG3	2.16	0.45
2:B:152:TYR:HB2	2:B:631:TRP:CD1	2.51	0.45
2:B:107:PHE:HB2	2:B:111:GLN:HG2	1.97	0.45
1:A:592:MET:N	1:A:593:PRO:HD2	2.31	0.45
1:A:489:ASN:HD21	1:A:511:LEU:N	2.15	0.45
2:B:36:ILE:HB	2:B:205:ILE:HG12	1.99	0.45
2:B:1070:ASP:OD1	2:B:1071:GLY:N	2.49	0.45
1:A:553:LYS:NZ	1:A:601:GLU:OE2	2.43	0.45
1:A:163:GLU:OE1	1:A:167:ARG:NH2	2.44	0.45
1:A:1090:TYR:HD1	1:A:1090:TYR:C	2.19	0.45
1:A:1150:GLU:HB3	2:B:49:TYR:OH	2.16	0.45
2:B:986:LEU:HD21	2:B:1003:PRO:HB3	1.97	0.45
1:A:249:GLY:HA2	1:A:301:LEU:HD22	1.99	0.45
1:A:1092:LYS:HB3	1:A:1094:LEU:HD12	1.99	0.45
2:B:673:ASP:HB2	2:B:677:LYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:THR:HG21	1:A:433:LEU:HD13	1.99	0.45
2:B:128:THR:HG23	2:B:184:GLU:HG3	1.99	0.45
1:A:1194:LYS:O	1:A:1198:GLU:HB2	2.17	0.44
2:B:190:LEU:O	2:B:194:ILE:HG13	2.17	0.44
1:A:939:HIS:HD2	1:A:941:ASP:H	1.66	0.44
2:B:632:LEU:HD23	2:B:632:LEU:HA	1.86	0.44
1:A:1129:GLU:O	1:A:1131:PRO:HD3	2.16	0.44
2:B:1045:GLN:HG3	2:B:1049:ARG:HD2	2.00	0.44
2:B:868:ALA:HB3	2:B:869:PRO:HD3	1.99	0.44
1:A:804:VAL:HB	1:A:874:ALA:HB2	1.99	0.44
1:A:447:ARG:HH21	3:X:54:DG:H1'	1.82	0.44
1:A:1112:PHE:CD1	1:A:1112:PHE:N	2.84	0.44
2:B:495:ALA:HB1	2:B:500:GLU:HG3	1.99	0.44
1:A:376:LEU:O	1:A:380:THR:HG23	2.18	0.44
1:A:481:ARG:HD3	1:A:523:THR:HG21	2.00	0.44
1:A:558:GLU:HG2	1:A:879:PHE:CE1	2.52	0.44
1:A:93:HIS:O	1:A:97:GLN:HG2	2.18	0.44
2:B:505:LEU:O	2:B:508:TYR:HB3	2.17	0.44
1:A:268:ILE:HA	1:A:271:GLN:HG3	1.99	0.44
2:B:309:GLN:HB2	2:B:695:HIS:CE1	2.53	0.44
1:A:574:LYS:HB3	1:A:576:THR:HG22	1.99	0.44
1:A:553:LYS:HD2	1:A:959:LEU:HB3	1.99	0.44
1:A:1186:PHE:O	1:A:1190:ALA:N	2.45	0.44
1:A:682:ASP:N	1:A:682:ASP:OD1	2.51	0.44
1:A:496:MET:HG3	1:A:501:GLY:HA3	1.99	0.44
1:A:271:GLN:HA	1:A:277:LEU:HD11	2.00	0.43
2:B:485:LEU:HA	2:B:485:LEU:HD12	1.88	0.43
2:B:525:ALA:HB3	2:B:534:ALA:HB2	1.99	0.43
1:A:1081:GLU:HA	1:A:1084:GLN:NE2	2.33	0.43
1:A:99:SER:O	1:A:102:ASN:ND2	2.51	0.43
3:X:41:DC:H2"	3:X:42:DG:C8	2.53	0.43
1:A:706:LYS:HA	1:A:706:LYS:HD3	1.77	0.43
2:B:515:PRO:HG3	2:B:541:TRP:CH2	2.54	0.43
1:A:367:ASP:HB2	1:A:370:ASP:CG	2.39	0.43
1:A:857:ARG:HG3	1:A:911:TYR:HE1	1.83	0.43
1:A:189:ARG:NH1	1:A:370:ASP:OD1	2.42	0.43
1:A:202:VAL:HG12	1:A:343:GLU:HG2	2.00	0.43
1:A:15:GLN:O	1:A:19:ILE:HG13	2.19	0.43
2:B:261[B]:ARG:HG2	2:B:261[B]:ARG:NH1	2.33	0.43
1:A:56:ASP:HA	1:A:97:GLN:OE1	2.19	0.43
1:A:1190:ALA:HB3	1:A:1191:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1107:ARG:NH2	2:B:1111:GLU:OE2	2.51	0.43
2:B:398:TRP:CH2	2:B:485:LEU:HB3	2.53	0.43
2:B:445:LYS:O	2:B:478:ARG:NH2	2.52	0.43
3:X:61:DT:H6	3:X:61:DT:H2'	1.63	0.42
1:A:118:LYS:HB3	2:B:621:ASN:ND2	2.34	0.42
1:A:339:LYS:HB3	1:A:340:PRO:HD3	2.01	0.42
2:B:24:ASP:HA	2:B:27:ARG:HD2	2.01	0.42
1:A:1193:LEU:HD13	1:A:1223:PHE:CZ	2.54	0.42
1:A:136:THR:HG21	1:A:768:MET:HG3	2.01	0.42
1:A:1077:PRO:CD	1:A:1112:PHE:HD2	2.32	0.42
2:B:841:LEU:HD21	2:B:851:LEU:HD21	2.01	0.42
1:A:567:PHE:HB3	1:A:580:ILE:CG1	2.49	0.42
2:B:729:GLN:O	2:B:739:ILE:HG21	2.20	0.42
1:A:1053:LYS:H	1:A:1053:LYS:HG2	1.70	0.42
2:B:68:PHE:HB3	2:B:187:LEU:HD11	2.01	0.42
1:A:663:LEU:HD23	1:A:663:LEU:HA	1.92	0.42
1:A:326:ARG:HG2	2:B:1021:PRO:HG3	2.00	0.42
1:A:634:ASP:OD1	2:B:408:LYS:HE2	2.20	0.42
2:B:1110:ILE:HD13	2:B:1130:CYS:HB2	2.01	0.42
1:A:864:LEU:HA	1:A:864:LEU:HD12	1.71	0.42
1:A:479:ARG:HB2	1:A:800:GLU:OE1	2.20	0.42
2:B:787:ARG:HG3	2:B:787:ARG:NH1	2.29	0.42
1:A:753:THR:CG2	1:A:754:ALA:N	2.82	0.42
1:A:29:ALA:O	1:A:473:ASP:HA	2.19	0.42
2:B:533:GLU:O	2:B:536:GLN:HG2	2.20	0.42
1:A:707:ASN:OD1	1:A:707:ASN:N	2.51	0.42
2:B:548:LEU:O	2:B:552:VAL:HG13	2.20	0.42
1:A:276:GLU:CG	1:A:280:ARG:HE	2.27	0.42
3:X:68:DT:H6	3:X:68:DT:H5'	1.83	0.42
1:A:63:VAL:HG22	1:A:406:VAL:HG22	2.01	0.42
1:A:886:ASP:OD2	1:A:889:LYS:HB2	2.19	0.42
1:A:42:GLU:HA	1:A:45:ILE:HD12	2.02	0.41
1:A:570:TYR:CE2	1:A:572:GLY:HA2	2.54	0.41
1:A:517:TYR:HA	1:A:518:PRO:HD2	1.91	0.41
1:A:1194:LYS:HB2	1:A:1230:LEU:HD21	2.02	0.41
1:A:339:LYS:O	1:A:343:GLU:HG3	2.20	0.41
1:A:550:PHE:CZ	1:A:956:SER:HB3	2.55	0.41
2:B:327:ILE:HD13	2:B:607:LEU:HD11	2.01	0.41
1:A:711:SER:HB2	1:A:744:TYR:CE1	2.55	0.41
1:A:40:LEU:HG	1:A:405:LEU:HD23	2.02	0.41
1:A:927:HIS:HD2	1:A:929:ASP:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:VAL:HG13	1:A:758:LEU:HA	2.02	0.41
1:A:208:SER:OG	1:A:209:GLU:N	2.54	0.41
2:B:338:LYS:N	2:B:338:LYS:HD2	2.35	0.41
1:A:37:THR:O	1:A:41:VAL:HG23	2.20	0.41
1:A:1000:TRP:HB2	2:B:336:ARG:HH11	1.86	0.41
1:A:803:VAL:HG22	1:A:877:LYS:HB2	2.02	0.41
1:A:607:ILE:HA	1:A:608:PRO:HD3	1.90	0.41
2:B:163:HIS:O	2:B:166:SER:OG	2.33	0.41
2:B:953:LYS:HG2	2:B:953:LYS:H	1.54	0.41
1:A:1065:HIS:O	1:A:1069:GLN:HG2	2.21	0.41
1:A:608:PRO:HB2	1:A:787:VAL:HG12	2.02	0.41
1:A:781:LEU:HD12	1:A:781:LEU:H	1.85	0.41
1:A:1049:PHE:CD1	2:B:552:VAL:HG21	2.56	0.41
1:A:710:VAL:HG11	1:A:761:PHE:CD2	2.56	0.41
1:A:568:LYS:HD2	1:A:568:LYS:HA	1.72	0.41
1:A:675:LYS:HB3	1:A:675:LYS:HE2	1.93	0.41
1:A:12:THR:HB	1:A:15:GLN:HG3	2.03	0.41
3:X:46:DT:H2"	3:X:47:DA:H8	1.85	0.41
1:A:629:VAL:HG11	1:A:717:VAL:HG11	2.03	0.40
2:B:618:PRO:HD3	2:B:647:LEU:HG	2.03	0.40
2:B:497:THR:HA	2:B:559:GLU:HA	2.03	0.40
2:B:219:ARG:NH1	2:B:223:GLN:OE1	2.53	0.40
2:B:1068:LYS:HG2	2:B:1074:ARG:HB3	2.04	0.40
1:A:561:LYS:HE2	1:A:561:LYS:HB3	1.90	0.40
2:B:487:GLN:HG2	2:B:491:ARG:HD2	2.03	0.40
1:A:519:ASP:O	1:A:520:ASN:ND2	2.54	0.40
1:A:657:GLU:O	1:A:661:ILE:HG13	2.22	0.40
1:A:139:GLU:HB3	1:A:771:ARG:NH2	2.36	0.40
2:B:189:LEU:HA	2:B:189:LEU:HD12	1.94	0.40
2:B:315:MET:O	2:B:668:SER:HA	2.20	0.40
2:B:1152:ILE:O	2:B:1156:ILE:HG13	2.21	0.40
1:A:860:LEU:HA	1:A:860:LEU:HD12	1.80	0.40
2:B:464:THR:O	2:B:468:ILE:HG13	2.22	0.40
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.94	0.40
2:B:73:TRP:O	2:B:77:GLN:HG2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1167/1232 (95%)	1137 (97%)	29 (2%)	1 (0%)	56 90
2	B	1153/1166 (99%)	1120 (97%)	31 (3%)	2 (0%)	52 88
All	All	2320/2398 (97%)	2257 (97%)	60 (3%)	3 (0%)	56 90

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	177	ALA
1	A	592	MET
2	B	1043	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	1019/1062 (96%)	944 (93%)	75 (7%)	17 52
2	B	1022/1029 (99%)	952 (93%)	70 (7%)	20 56
All	All	2041/2091 (98%)	1896 (93%)	145 (7%)	18 54

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	24	GLN
1	A	46	ARG

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Mol	Chain	Res	Type
1	A	47	LYS
1	A	73	MET
1	A	102	ASN
1	A	115	GLN
1	A	178	GLN
1	A	189	ARG
1	A	208	SER
1	A	317	GLU
1	A	361	GLN
1	A	371	LEU
1	A	399	GLU
1	A	447	ARG
1	A	448	LEU
1	A	464	SER
1	A	479	ARG
1	A	483	ASP
1	A	499	LYS
1	A	502	GLU
1	A	527	LEU
1	A	545	LEU
1	A	551	GLU
1	A	558	GLU
1	A	568	LYS
1	A	573	LYS
1	A	574	LYS
1	A	580	ILE
1	A	590	ARG
1	A	627	LEU
1	A	659	SER
1	A	660	LEU
1	A	672	GLU
1	A	710	VAL
1	A	746	ARG
1	A	753	THR
1	A	762	LEU
1	A	767	ARG
1	A	771	ARG
1	A	779	ARG
1	A	781	LEU
1	A	789	ARG
1	A	797	LYS
1	A	821	SER

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Mol	Chain	Res	Type
1	A	823	LEU
1	A	826	LYS
1	A	852	LYS
1	A	860	LEU
1	A	902	ASP
1	A	956	SER
1	A	959	LEU
1	A	967	ARG
1	A	1014	GLN
1	A	1046	ARG
1	A	1053	LYS
1	A	1056	THR
1	A	1059	GLU
1	A	1065	HIS
1	A	1066	THR
1	A	1067	VAL
1	A	1069	GLN
1	A	1070	HIS
1	A	1080	GLU
1	A	1084	GLN
1	A	1088	ARG
1	A	1090	TYR
1	A	1094	LEU
1	A	1101	ASP
1	A	1103	ILE
1	A	1129	GLU
1	A	1152	LEU
1	A	1177	ARG
1	A	1179	GLU
1	A	1181	LYS
2	B	37	PHE
2	B	42	GLN
2	B	60	MET
2	B	69	SER
2	B	74	ARG
2	B	96	LEU
2	B	122	GLN
2	B	146	SER
2	B	148	THR
2	B	169	TYR
2	B	183	SER
2	B	207	VAL

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Mol	Chain	Res	Type
2	B	218	PHE
2	B	261[A]	ARG
2	B	261[B]	ARG
2	B	265	LYS
2	B	275	TYR
2	B	286	LYS
2	B	332	HIS
2	B	353	GLU
2	B	445	LYS
2	B	447	ASP
2	B	460	ASP
2	B	465	ASP
2	B	510	GLU
2	B	528	ASP
2	B	530	ARG
2	B	535	GLN
2	B	551	PHE
2	B	563	ASP
2	B	570	GLU
2	B	590	VAL
2	B	594	ASP
2	B	598	MET
2	B	617	ARG
2	B	619	ASP
2	B	635	ILE
2	B	641	SER
2	B	644	ARG
2	B	647	LEU
2	B	651	HIS
2	B	673	ASP
2	B	701	THR
2	B	756	ARG
2	B	758	GLN
2	B	777	ARG
2	B	780	SER
2	B	781	ARG
2	B	862	ASP
2	B	873	LYS
2	B	877	LEU
2	B	887	GLU
2	B	927	LEU
2	B	940	VAL

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Mol	Chain	Res	Type
2	B	953	LYS
2	B	964	SER
2	B	1017	GLN
2	B	1020	LEU
2	B	1044	ASP
2	B	1056	GLN
2	B	1063	ILE
2	B	1073	LEU
2	B	1084	GLU
2	B	1085	PHE
2	B	1101	GLU
2	B	1104	THR
2	B	1122	THR
2	B	1127	LYS
2	B	1139	ASN
2	B	1148	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	183	GLN
1	A	520	ASN
1	A	577	HIS
1	A	579	ASN
1	A	612	ASN
1	A	749	GLN
1	A	794	HIS
1	A	819	ASN
1	A	927	HIS
1	A	939	HIS
1	A	1069	GLN
1	A	1084	GLN
1	A	1110	GLN
1	A	1202	GLN
2	B	122	GLN
2	B	264	GLN
2	B	332	HIS
2	B	487	GLN
2	B	621	ASN
2	B	729	GLN

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

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	ANP	A	2233	5	27,33,33	1.18	4 (14%)	30,52,52	0.98	3 (10%)
6	SF4	B	2160	2	0,12,12	0.00	-	0,24,24	0.00	-
4	ANP	B	2161	5	27,33,33	1.15	4 (14%)	30,52,52	1.04	2 (6%)

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
4	ANP	A	2233	5	-	0/12/38/38	0/3/3/3
6	SF4	B	2160	2	-	0/0/48/48	0/6/5/5
4	ANP	B	2161	5	-	0/12/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2161	ANP	PB-O3A	-2.70	1.55	1.59
4	A	2233	ANP	PB-O3A	-2.66	1.55	1.59
4	B	2161	ANP	C8-N7	-2.25	1.30	1.34
4	A	2233	ANP	C8-N7	-2.07	1.30	1.34
4	B	2161	ANP	PG-N3B	2.28	1.69	1.63
4	A	2233	ANP	PG-N3B	2.35	1.69	1.63
4	A	2233	ANP	PG-O1G	3.03	1.49	1.46
4	B	2161	ANP	PG-O1G	3.22	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2161	ANP	PA-O3A-PB	-3.16	122.07	132.67
4	A	2233	ANP	PA-O3A-PB	-2.82	123.22	132.67
4	B	2161	ANP	O1G-PG-N3B	-2.73	107.71	111.90
4	A	2233	ANP	O3G-PG-O1G	-2.04	108.07	113.49
4	A	2233	ANP	C4-C5-N7	2.19	111.49	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2233	ANP	2	0
6	B	2160	SF4	1	0
4	B	2161	ANP	5	0

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, 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	1177/1232 (95%)	-0.11	36 (3%) 52 24	35, 79, 137, 163	0
2	B	1156/1166 (99%)	-0.24	7 (0%) 90 73	33, 76, 120, 142	0
3	X	46/70 (65%)	0.57	4 (8%) 13 4	67, 143, 166, 176	0
All	All	2379/2468 (96%)	-0.16	47 (1%) 68 39	33, 78, 132, 176	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	930	GLN	4.7
1	A	293	LYS	3.9
1	A	1183	GLN	3.7
2	B	1116	LYS	3.7
1	A	1054	GLY	3.7
1	A	1184	HIS	3.6
1	A	1110	GLN	3.6
3	X	38	DG	3.5
1	A	87	GLN	3.5
2	B	282	GLU	3.5
1	A	1178	ILE	3.4
1	A	1060	LYS	3.4
1	A	1055	LEU	3.3
1	A	247	PRO	3.3
2	B	1115	MET	3.2
1	A	959	LEU	3.1
1	A	292	VAL	3.0
1	A	288	ARG	3.0
1	A	1102	ALA	2.9
2	B	1123	TYR	2.9
3	X	39	DC	2.8
1	A	291	ALA	2.8
1	A	302	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1056	THR	2.8
1	A	290	LYS	2.6
1	A	1094	LEU	2.6
1	A	960	LEU	2.6
1	A	1169	TYR	2.6
1	A	301	LEU	2.5
3	X	18	DC	2.4
1	A	968	MET	2.4
2	B	1143	PRO	2.3
2	B	1118	LYS	2.3
1	A	556	ALA	2.2
1	A	1059	GLU	2.2
1	A	1182	PHE	2.1
1	A	970	GLU	2.1
3	X	49	DA	2.1
1	A	1147	GLU	2.1
1	A	1112	PHE	2.1
1	A	784	GLN	2.1
1	A	286	PHE	2.1
1	A	386	GLY	2.1
1	A	1148	ALA	2.1
1	A	528	LEU	2.1
1	A	306	THR	2.0
1	A	1096	THR	2.0

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

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	ANP	B	2161	31/31	0.86	0.23	-0.16	60,89,109,111	0
4	ANP	A	2233	31/31	0.89	0.21	-0.52	64,84,94,97	0
6	SF4	B	2160	8/8	0.98	0.07	-2.61	86,113,125,125	0
5	MG	B	2162	1/1	0.96	0.21	-	78,78,78,78	0
5	MG	A	2234	1/1	0.93	0.15	-	85,85,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.