



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:23 pm GMT

PDB ID : 3GPL
Title : Crystal structure of the ternary complex of RecD2 with DNA and ADPNP
Authors : Saikrishnan, K.; Cook, N.; Wigley, D.B.
Deposited on : 2009-03-23
Resolution : 2.50 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

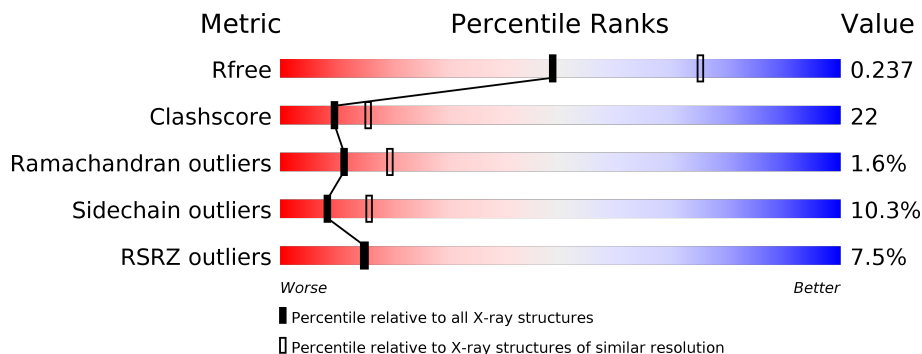
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	574	<div> <div>6%</div> <div>58%</div> <div>26%</div> <div>6%</div> <div>10%</div> </div>
1	B	574	<div> <div>7%</div> <div>57%</div> <div>27%</div> <div>6%</div> <div>10%</div> </div>
2	X	8	<div> <div>13%</div> <div>75%</div> <div>13%</div> </div>
2	Y	8	<div> <div>13%</div> <div>75%</div> <div>13%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8322 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 Exodeoxyribonuclease V, subunit RecD, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	2	0
			3899	2447	720	722	10			
1	B	516	Total	C	N	O	S	0	2	0
			3899	2447	720	722	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	MET	-	EXPRESSION TAG	UNP Q9RT63
A	716	LEU	-	EXPRESSION TAG	UNP Q9RT63
A	717	GLU	-	EXPRESSION TAG	UNP Q9RT63
A	718	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	719	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	720	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	721	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	722	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	723	HIS	-	EXPRESSION TAG	UNP Q9RT63
B	150	MET	-	EXPRESSION TAG	UNP Q9RT63
B	716	LEU	-	EXPRESSION TAG	UNP Q9RT63
B	717	GLU	-	EXPRESSION TAG	UNP Q9RT63
B	718	HIS	-	EXPRESSION TAG	UNP Q9RT63
B	719	HIS	-	EXPRESSION TAG	UNP Q9RT63
B	720	HIS	-	EXPRESSION TAG	UNP Q9RT63
B	721	HIS	-	EXPRESSION TAG	UNP Q9RT63
B	722	HIS	-	EXPRESSION TAG	UNP Q9RT63
B	723	HIS	-	EXPRESSION TAG	UNP Q9RT63

- Molecule 2 is a DNA chain called 5'-D(*T*TP*TP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	7	Total	C	N	O	P	1	0	0
			137	70	14	47	6			

Continued on next page...

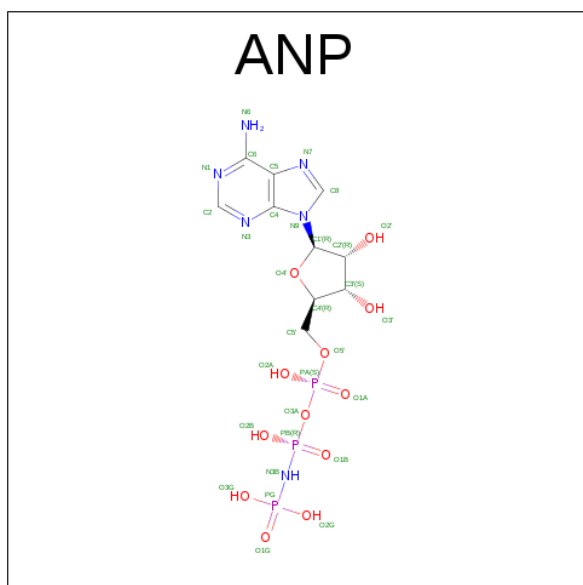
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	7	Total	C	N	O	P	1	0	0
			137	70	14	47	6			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	94	Total	O	0	0
			94	94		

Continued on next page...

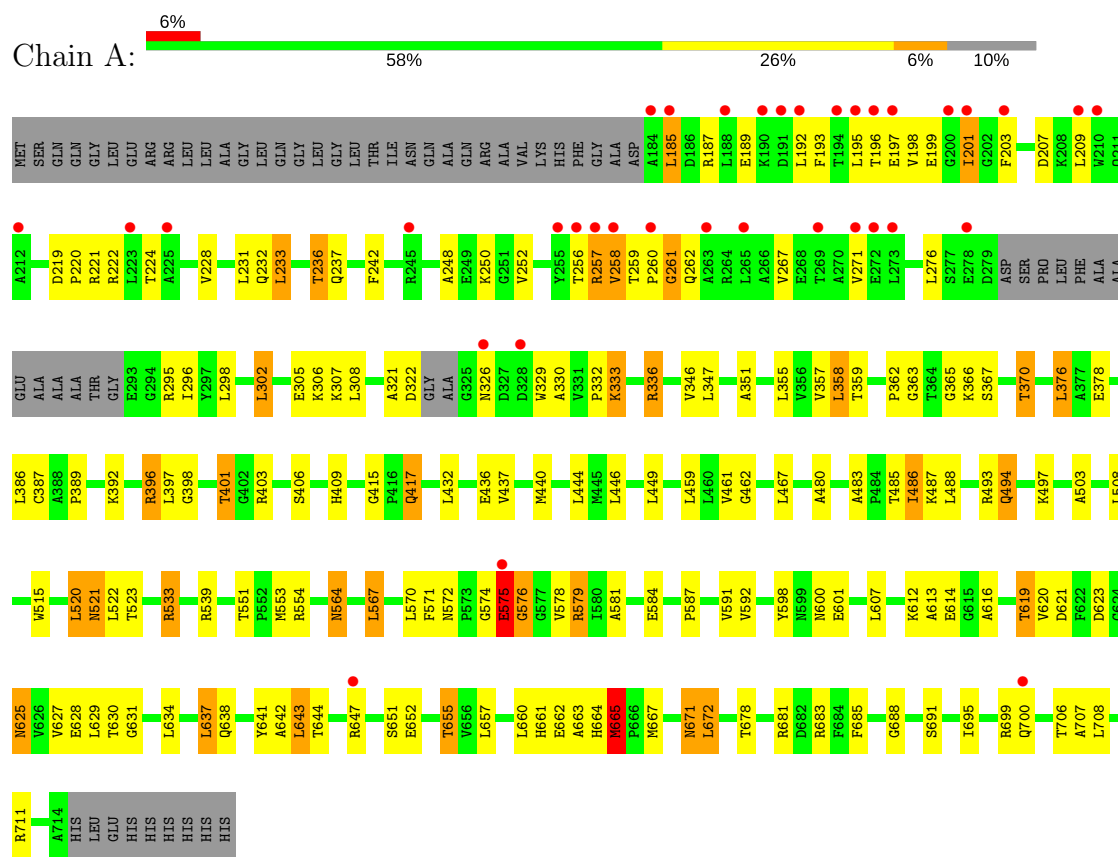
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	76	Total 76	O 76	0	0
5	X	9	Total 9	O 9	0	0
5	Y	7	Total 7	O 7	0	0

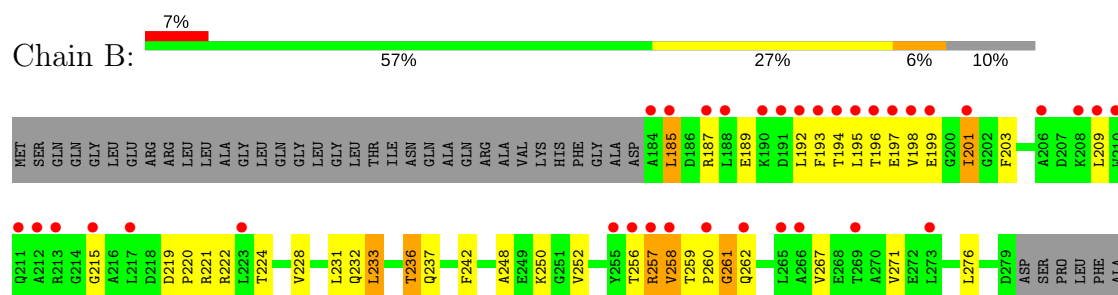
3 Residue-property plots [i](#)

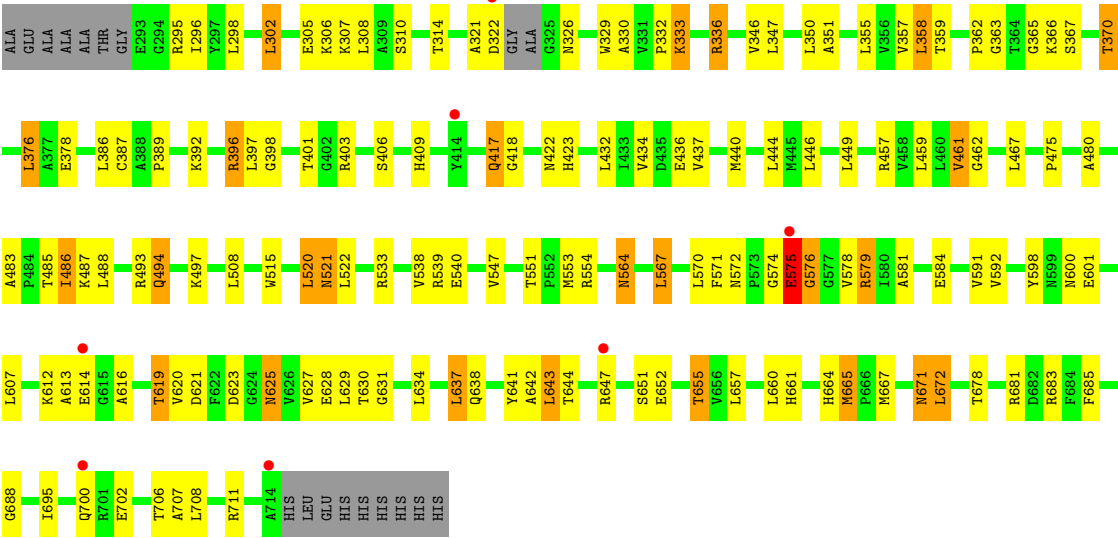
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Exodeoxyribonuclease V, subunit RecD, putative

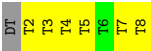


- Molecule 1: Exodeoxyribonuclease V, subunit RecD, putative

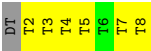
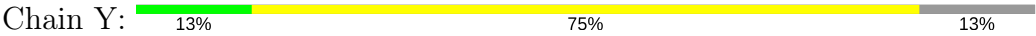




● Molecule 2: 5'-D(*T*TP*TP*TP*TP*TP*TP*T)-3'



● Molecule 2: 5'-D(*T*TP*TP*TP*TP*TP*TP*T)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.12Å 130.36Å 80.05Å 90.00° 107.34° 90.00°	Depositor
Resolution (Å)	43.27 – 2.50 43.27 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.27-2.50) 98.5 (43.27-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.232 , 0.273 0.235 , 0.237	Depositor DCC
R_{free} test set	2200 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8322	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: MG, ANP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/3975	0.63	3/5395 (0.1%)
1	B	0.35	0/3975	0.63	3/5395 (0.1%)
2	X	0.39	0/150	1.02	0/230
2	Y	0.39	0/150	1.03	0/230
All	All	0.35	0/8250	0.65	6/11250 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	574	GLY	N-CA-C	5.81	127.61	113.10
1	A	574	GLY	N-CA-C	5.75	127.49	113.10
1	B	298	LEU	N-CA-C	-5.23	96.89	111.00
1	B	575	GLU	N-CA-C	5.14	124.88	111.00
1	A	298	LEU	N-CA-C	-5.11	97.20	111.00
1	A	575	GLU	N-CA-C	5.09	124.74	111.00

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	3899	0	3959	172	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3899	0	3959	174	0
2	X	137	0	86	7	0
2	Y	137	0	86	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	13	3	0
4	B	31	0	13	4	0
5	A	94	0	0	9	0
5	B	76	0	0	10	0
5	X	9	0	0	2	0
5	Y	7	0	0	0	0
All	All	8322	0	8116	350	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 22.

All (350) 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:579:ARG:HB3	1:B:579:ARG:HH11	1.28	0.99
1:A:357:VAL:HB	1:A:485:THR:HG22	1.43	0.98
1:B:357:VAL:HB	1:B:485:THR:HG22	1.45	0.97
1:A:579:ARG:HB3	1:A:579:ARG:HH11	1.27	0.96
1:A:258:VAL:HB	1:A:262:GLN:HE21	1.35	0.92
1:B:258:VAL:HB	1:B:262:GLN:HE21	1.35	0.91
1:A:333:LYS:HE3	1:A:333:LYS:HA	1.54	0.90
1:B:655:THR:HG21	1:B:683:ARG:HH21	1.38	0.88
1:B:591:VAL:HG11	1:B:637:LEU:HD22	1.57	0.85
1:A:655:THR:HG21	1:A:683:ARG:HH21	1.42	0.84
1:A:665:MET:HE1	1:A:695:ILE:HD13	1.59	0.84
1:A:591:VAL:HG11	1:A:637:LEU:HD22	1.59	0.84
1:A:258:VAL:HB	1:A:262:GLN:NE2	1.93	0.83
1:B:333:LYS:HE3	1:B:333:LYS:HA	1.58	0.83
1:B:258:VAL:HB	1:B:262:GLN:NE2	1.93	0.83
1:B:665:MET:HE1	1:B:695:ILE:HD13	1.60	0.83
1:A:231:LEU:HD21	1:A:296:ILE:HD11	1.61	0.82
1:A:564:ASN:HD21	1:A:642:ALA:H	1.28	0.82
1:A:267:VAL:O	1:A:271:VAL:HG23	1.80	0.82
1:B:564:ASN:HD21	1:B:642:ALA:H	1.28	0.81
1:B:231:LEU:HD21	1:B:296:ILE:HD11	1.62	0.79
1:A:196:THR:HG23	1:A:203:PHE:HB2	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:THR:HG23	1:B:403:ARG:H	1.48	0.79
1:B:196:THR:HG23	1:B:203:PHE:HB2	1.63	0.78
1:B:267:VAL:O	1:B:271:VAL:HG23	1.82	0.78
1:A:236:THR:CG2	1:A:237:GLN:HE21	1.96	0.78
1:B:236:THR:CG2	1:B:237:GLN:HE21	1.97	0.78
1:A:347:LEU:HG	1:A:376:LEU:HD12	1.68	0.76
1:B:307:LYS:HD2	1:B:446:LEU:HD11	1.67	0.76
1:B:193:PHE:CZ	1:B:222:ARG:HG3	2.20	0.76
1:A:193:PHE:CZ	1:A:222:ARG:HG3	2.20	0.76
1:A:307:LYS:HD2	1:A:446:LEU:HD11	1.67	0.75
1:B:347:LEU:HG	1:B:376:LEU:HD12	1.67	0.75
1:A:359:THR:HG22	1:A:462:GLY:O	1.87	0.74
1:A:706:THR:HG22	1:A:708:LEU:H	1.51	0.74
1:B:486:ILE:HD11	1:B:488:LEU:HD23	1.69	0.73
1:B:486:ILE:HD12	1:B:487:LYS:N	2.04	0.72
1:B:706:THR:HG22	1:B:708:LEU:H	1.53	0.72
1:B:359:THR:HG22	1:B:462:GLY:O	1.89	0.72
1:A:276:LEU:HD13	1:A:296:ILE:HD12	1.72	0.71
1:A:401:THR:HG23	1:A:403:ARG:H	1.55	0.71
1:A:508:LEU:CD1	1:B:250:LYS:HE3	2.20	0.71
1:A:486:ILE:HD11	1:A:488:LEU:HD23	1.73	0.71
1:A:553:MET:HE2	1:A:664:HIS:HA	1.71	0.71
1:A:486:ILE:HD12	1:A:487:LYS:N	2.07	0.70
1:B:553:MET:HE2	1:B:664:HIS:HA	1.73	0.70
1:A:306:LYS:HG3	1:A:711:ARG:HE	1.57	0.69
2:Y:2:DT:H2''	2:Y:3:DT:O5'	1.93	0.69
1:B:236:THR:HG22	1:B:237:GLN:HE21	1.57	0.69
1:A:612:LYS:HE2	1:A:614:GLU:CD	2.13	0.69
2:X:2:DT:H2''	2:X:3:DT:O5'	1.92	0.69
1:B:306:LYS:HG3	1:B:711:ARG:HE	1.57	0.68
1:B:612:LYS:HG2	1:B:619:THR:HG23	1.75	0.68
1:B:401:THR:HG23	1:B:403:ARG:N	2.07	0.68
1:B:497:LYS:NZ	1:B:497:LYS:H	1.92	0.68
1:A:523:THR:HG23	5:A:724:HOH:O	1.92	0.67
1:B:612:LYS:HE2	1:B:614:GLU:CD	2.15	0.67
1:B:276:LEU:HD13	1:B:296:ILE:HD12	1.75	0.67
1:B:396:ARG:HD3	1:B:651:SER:OG	1.94	0.67
1:A:612:LYS:HG2	1:A:619:THR:HG23	1.76	0.66
1:B:409:HIS:HD2	5:B:63:HOH:O	1.77	0.66
1:B:486:ILE:HD11	1:B:488:LEU:CD2	2.25	0.66
1:B:671:ASN:H	1:B:671:ASN:HD22	1.44	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:GLY:HA2	1:B:584:GLU:OE1	1.96	0.66
1:A:333:LYS:CE	1:A:336:ARG:HD3	2.26	0.66
1:B:367:SER:O	1:B:370:THR:HB	1.95	0.66
1:A:486:ILE:HD11	1:A:488:LEU:CD2	2.26	0.65
1:B:401:THR:CG2	1:B:403:ARG:H	2.09	0.65
1:A:236:THR:HG22	1:A:237:GLN:HE21	1.60	0.65
1:A:581:ALA:HB3	1:A:638:GLN:HG2	1.79	0.65
1:B:257:ARG:HB2	1:B:257:ARG:NH1	2.12	0.65
1:B:483:ALA:O	1:B:485:THR:HG23	1.97	0.65
1:A:579:ARG:CB	1:A:579:ARG:HH11	2.08	0.64
1:B:643:LEU:HD23	1:B:644:THR:H	1.62	0.64
1:A:401:THR:HG23	1:A:403:ARG:N	2.13	0.64
1:A:576:GLY:HA2	1:A:584:GLU:OE1	1.97	0.64
1:A:257:ARG:NH1	1:A:257:ARG:HB2	2.12	0.64
1:A:497:LYS:NZ	1:A:497:LYS:H	1.96	0.64
1:B:256:THR:O	1:B:257:ARG:HB2	1.98	0.63
1:A:367:SER:O	1:A:370:THR:HB	1.98	0.63
1:A:256:THR:O	1:A:257:ARG:HB2	1.98	0.63
1:B:581:ALA:HB3	1:B:638:GLN:HG2	1.79	0.63
1:A:333:LYS:HE3	1:A:336:ARG:HD3	1.81	0.63
1:A:396:ARG:HD3	1:A:651:SER:OG	1.98	0.63
1:B:256:THR:HG22	1:B:257:ARG:H	1.64	0.62
1:B:333:LYS:CE	1:B:336:ARG:HD3	2.27	0.62
1:B:671:ASN:HD22	1:B:671:ASN:N	1.97	0.62
1:A:661:HIS:H	1:A:664:HIS:HD2	1.47	0.62
1:A:256:THR:HG22	1:A:257:ARG:H	1.63	0.62
1:B:333:LYS:HE3	1:B:336:ARG:HD3	1.80	0.62
1:B:647[A]:ARG:HD3	2:Y:5:DT:OP1	1.99	0.62
5:B:79:HOH:O	2:Y:7:DT:H71	1.99	0.61
1:A:539:ARG:HG2	1:A:539:ARG:HH11	1.66	0.61
1:B:378:GLU:OE1	1:B:403:ARG:NE	2.22	0.61
1:B:570:LEU:HD12	1:B:571:PHE:CZ	2.36	0.60
1:A:256:THR:HG22	1:A:257:ARG:N	2.17	0.60
1:A:643:LEU:HD23	1:A:644:THR:H	1.66	0.60
1:B:539:ARG:HH11	1:B:539:ARG:HG2	1.66	0.60
1:A:570:LEU:HD12	1:A:571:PHE:CZ	2.37	0.59
1:B:422:ASN:HA	5:B:76:HOH:O	2.02	0.59
1:B:553:MET:HG2	1:B:667:MET:HG3	1.85	0.59
1:A:483:ALA:O	1:A:485:THR:HG23	2.02	0.59
1:B:256:THR:HG22	1:B:257:ARG:N	2.17	0.59
1:A:386:LEU:HD23	1:A:397:LEU:HD11	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:THR:CG2	1:A:403:ARG:H	2.14	0.59
1:B:661:HIS:H	1:B:664:HIS:HD2	1.50	0.58
1:A:619:THR:HB	1:A:628:GLU:HG2	1.86	0.58
1:A:671:ASN:HD22	1:A:671:ASN:H	1.51	0.58
1:B:417:GLN:HG3	5:B:81:HOH:O	2.03	0.58
1:B:386:LEU:HD23	1:B:397:LEU:HD11	1.85	0.58
1:A:553:MET:HG2	1:A:667:MET:HG3	1.85	0.58
1:A:671:ASN:HD22	1:A:671:ASN:N	2.01	0.57
1:B:564:ASN:ND2	1:B:642:ALA:H	1.99	0.57
1:B:643:LEU:HD21	1:B:647[B]:ARG:HB2	1.87	0.57
1:A:575:GLU:O	1:A:576:GLY:C	2.42	0.57
1:B:321:ALA:HB1	1:B:326:ASN:H	1.70	0.57
1:A:409:HIS:HD2	5:A:138:HOH:O	1.88	0.57
2:Y:2:DT:H2''	2:Y:3:DT:C5'	2.34	0.57
1:B:575:GLU:O	1:B:576:GLY:C	2.43	0.57
1:B:579:ARG:CB	1:B:579:ARG:HH11	2.11	0.57
1:B:702:GLU:HA	5:B:724:HOH:O	2.05	0.57
1:A:521:ASN:HD22	1:A:522:LEU:H	1.51	0.57
1:A:647[A]:ARG:HD3	2:X:5:DT:OP1	2.04	0.57
1:B:521:ASN:HD22	1:B:522:LEU:H	1.52	0.56
1:A:497:LYS:HZ3	1:A:497:LYS:H	1.54	0.56
1:A:564:ASN:ND2	1:A:642:ALA:H	1.98	0.56
1:A:199:GLU:O	1:A:201:ILE:HD13	2.05	0.56
1:A:321:ALA:HB1	1:A:326:ASN:H	1.71	0.56
1:B:619:THR:HB	1:B:628:GLU:HG2	1.86	0.56
2:X:2:DT:H2''	2:X:3:DT:C5'	2.35	0.56
1:A:250:LYS:HE3	1:B:508:LEU:CD1	2.36	0.56
1:B:199:GLU:O	1:B:201:ILE:HD13	2.04	0.56
1:B:259:THR:O	1:B:261:GLY:N	2.39	0.56
1:A:330:ALA:O	1:A:332:PRO:HD3	2.06	0.55
1:B:362:PRO:HG3	1:B:678:THR:HG21	1.88	0.55
1:B:248:ALA:O	1:B:252:VAL:HG23	2.07	0.55
1:B:363:GLY:H	4:B:801:ANP:HNB1	1.55	0.55
1:B:493:ARG:NH2	4:B:801:ANP:O2G	2.33	0.55
1:B:330:ALA:O	1:B:332:PRO:HD3	2.07	0.54
1:B:570:LEU:HD12	1:B:571:PHE:CE1	2.43	0.54
1:B:306:LYS:CG	1:B:711:ARG:HE	2.21	0.54
2:X:7:DT:H71	5:X:122:HOH:O	2.06	0.54
1:A:533:ARG:HG3	5:A:725:HOH:O	2.05	0.54
1:B:521:ASN:ND2	1:B:522:LEU:H	2.06	0.54
1:B:193:PHE:CE1	1:B:222:ARG:HG3	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LEU:HD23	1:A:641:TYR:HB3	1.90	0.54
1:A:521:ASN:ND2	1:A:522:LEU:H	2.05	0.54
1:A:570:LEU:HD12	1:A:571:PHE:CE1	2.43	0.54
1:A:306:LYS:CG	1:A:711:ARG:HE	2.20	0.54
1:A:236:THR:CG2	1:A:237:GLN:NE2	2.70	0.53
1:A:486:ILE:C	1:A:486:ILE:HD12	2.29	0.53
1:B:387:CYS:HA	1:B:406:SER:O	2.08	0.53
1:B:579:ARG:HB3	1:B:579:ARG:NH1	2.12	0.53
1:A:259:THR:O	1:A:261:GLY:N	2.40	0.53
1:A:201:ILE:H	1:A:201:ILE:HD13	1.72	0.53
1:B:486:ILE:HD12	1:B:486:ILE:C	2.28	0.53
1:A:362:PRO:HG3	1:A:678:THR:HG21	1.90	0.53
1:A:248:ALA:O	1:A:252:VAL:HG23	2.09	0.53
1:A:493:ARG:HG3	1:A:681:ARG:HG2	1.91	0.53
1:B:236:THR:HG22	1:B:237:GLN:NE2	2.24	0.52
1:B:643:LEU:CD2	1:B:647[B]:ARG:HB2	2.39	0.52
1:A:193:PHE:CE1	1:A:222:ARG:HG3	2.44	0.52
1:A:647[A]:ARG:HG2	5:X:9:HOH:O	2.09	0.52
1:A:386:LEU:HB3	1:A:397:LEU:CD1	2.39	0.52
1:A:387:CYS:HA	1:A:406:SER:O	2.10	0.52
1:B:362:PRO:HA	4:B:801:ANP:O3G	2.10	0.52
1:A:329:TRP:CD1	1:A:351:ALA:HB2	2.45	0.51
1:B:578:VAL:HG23	1:B:613:ALA:HB1	1.92	0.51
1:B:567:LEU:HD23	1:B:641:TYR:HB3	1.92	0.51
1:B:660:LEU:O	1:B:688:GLY:HA3	2.11	0.51
1:A:643:LEU:HD21	1:A:647[B]:ARG:HB2	1.93	0.51
1:B:201:ILE:HD13	1:B:201:ILE:H	1.75	0.51
1:B:497:LYS:HZ2	1:B:497:LYS:H	1.59	0.51
1:B:625:ASN:HD22	1:B:625:ASN:C	2.13	0.51
1:B:643:LEU:HD23	1:B:644:THR:N	2.25	0.51
1:A:236:THR:HG22	1:A:237:GLN:HG2	1.93	0.50
1:A:467:LEU:HD21	1:A:672:LEU:HA	1.93	0.50
1:A:625:ASN:C	1:A:625:ASN:HD22	2.13	0.50
1:A:578:VAL:HG23	1:A:613:ALA:HB1	1.92	0.50
1:B:497:LYS:HZ3	1:B:497:LYS:H	1.58	0.50
1:B:329:TRP:CD1	1:B:351:ALA:HB2	2.46	0.50
1:A:209:LEU:O	1:A:209:LEU:HD13	2.11	0.50
1:B:192:LEU:HD21	1:B:209:LEU:CD1	2.42	0.49
1:B:386:LEU:HB3	1:B:397:LEU:CD1	2.42	0.49
1:A:638:GLN:NE2	5:A:731:HOH:O	2.42	0.49
1:B:209:LEU:O	1:B:209:LEU:HD13	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:HG22	1:A:237:GLN:NE2	2.26	0.49
1:B:219:ASP:CG	1:B:221:ARG:HE	2.15	0.49
1:B:551:THR:O	1:B:644:THR:HA	2.13	0.49
1:B:657:LEU:HA	1:B:685:PHE:O	2.12	0.49
1:B:480:ALA:HA	1:B:485:THR:HG21	1.95	0.49
1:B:638:GLN:NE2	5:B:111:HOH:O	2.44	0.49
1:B:423:HIS:HB2	5:B:82:HOH:O	2.13	0.49
1:B:493:ARG:HG3	1:B:681:ARG:HG2	1.94	0.49
1:A:192:LEU:HD21	1:A:209:LEU:CD1	2.43	0.49
1:B:192:LEU:HD21	1:B:209:LEU:HD13	1.95	0.49
1:A:480:ALA:HA	1:A:485:THR:HG21	1.95	0.48
1:B:418:GLY:HA2	5:B:71:HOH:O	2.13	0.48
1:B:236:THR:CG2	1:B:237:GLN:NE2	2.71	0.48
1:A:224:THR:HG21	5:A:124:HOH:O	2.13	0.48
1:A:493:ARG:HD3	1:A:652:GLU:OE1	2.13	0.48
1:A:522:LEU:C	1:A:522:LEU:HD23	2.34	0.48
1:B:467:LEU:HD21	1:B:672:LEU:HA	1.96	0.48
1:A:657:LEU:HA	1:A:685:PHE:O	2.14	0.48
1:B:493:ARG:HD3	1:B:652:GLU:OE1	2.13	0.48
1:B:252:VAL:O	1:B:256:THR:HB	2.14	0.48
1:A:252:VAL:O	1:A:256:THR:HB	2.14	0.48
1:A:219:ASP:CG	1:A:221:ARG:HE	2.17	0.48
1:A:643:LEU:HD23	1:A:644:THR:N	2.28	0.48
1:B:575:GLU:H	1:B:575:GLU:CD	2.13	0.48
1:A:539:ARG:NH1	1:A:539:ARG:HG2	2.29	0.48
1:B:539:ARG:NH1	1:B:539:ARG:HG2	2.28	0.47
1:A:192:LEU:HD21	1:A:209:LEU:HD13	1.96	0.47
1:B:661:HIS:H	1:B:664:HIS:CD2	2.32	0.47
1:B:554:ARG:HG3	2:Y:4:DT:OP1	2.14	0.47
1:A:305:GLU:OE2	1:A:707:ALA:HB3	2.14	0.47
1:B:417:GLN:HA	1:B:417:GLN:HE21	1.80	0.47
1:A:551:THR:O	1:A:644:THR:HA	2.14	0.47
1:B:631:GLY:O	1:B:634:LEU:HB2	2.15	0.47
1:A:195:LEU:HA	1:A:198:VAL:HB	1.97	0.47
1:A:363:GLY:H	4:A:801:ANP:HNB1	1.63	0.46
1:A:699:ARG:CD	5:A:30:HOH:O	2.62	0.46
1:A:699:ARG:HD3	5:A:30:HOH:O	2.15	0.46
1:B:522:LEU:HD23	1:B:522:LEU:C	2.35	0.46
1:A:417:GLN:HA	1:A:417:GLN:HE21	1.81	0.46
1:A:508:LEU:HD11	1:B:250:LYS:HE3	1.97	0.46
1:B:378:GLU:CD	1:B:403:ARG:HH21	2.19	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:LYS:NZ	1:B:497:LYS:N	2.62	0.46
1:B:612:LYS:HG2	1:B:619:THR:CG2	2.45	0.46
1:A:370:THR:HG21	1:A:397:LEU:HD21	1.97	0.46
1:A:396:ARG:HB3	5:A:9:HOH:O	2.15	0.46
1:B:236:THR:HG22	1:B:237:GLN:HG2	1.97	0.46
1:A:378:GLU:OE1	1:A:403:ARG:NE	2.24	0.46
1:B:322:ASP:HB3	1:B:326:ASN:HB3	1.97	0.46
1:A:201:ILE:N	1:A:201:ILE:HD13	2.32	0.45
1:A:579:ARG:HB3	1:A:579:ARG:NH1	2.11	0.45
1:A:564:ASN:HD22	1:A:641:TYR:HB2	1.81	0.45
1:A:662:GLU:OE2	1:A:691:SER:OG	2.28	0.45
1:A:643:LEU:CD2	1:A:647[B]:ARG:HB2	2.46	0.45
1:A:660:LEU:O	1:A:688:GLY:HA3	2.16	0.45
1:A:392:LYS:HD3	1:A:643:LEU:HD11	1.97	0.45
1:A:494:GLN:NE2	1:A:494:GLN:H	2.15	0.45
1:B:643:LEU:HD21	1:B:647[B]:ARG:CB	2.46	0.45
1:A:220:PRO:O	1:A:224:THR:HG22	2.17	0.45
1:A:233:LEU:HA	1:A:233:LEU:HD12	1.84	0.45
1:A:322:ASP:HB3	1:A:326:ASN:HB3	1.98	0.45
1:A:389:PRO:HG3	1:A:440:MET:HG3	1.97	0.45
1:A:592:VAL:HG22	1:A:607:LEU:CD2	2.45	0.45
1:B:357:VAL:HB	1:B:485:THR:CG2	2.33	0.45
1:B:396:ARG:HB3	5:B:727:HOH:O	2.17	0.45
1:B:389:PRO:HG3	1:B:440:MET:HG3	1.99	0.45
1:A:365:GLY:HA2	4:A:801:ANP:O1A	2.17	0.45
1:A:616:ALA:O	1:A:630:THR:HG22	2.17	0.45
1:B:195:LEU:HA	1:B:198:VAL:HB	1.97	0.45
1:A:228:VAL:O	1:A:232:GLN:HG3	2.18	0.44
1:B:592:VAL:HG22	1:B:607:LEU:CD2	2.47	0.44
1:B:620:VAL:HG12	1:B:621:ASP:N	2.32	0.44
2:Y:2:DT:C2'	2:Y:3:DT:O5'	2.64	0.44
1:A:415:GLY:HA3	5:A:143:HOH:O	2.17	0.44
1:B:681:ARG:HG3	1:B:681:ARG:HH21	1.81	0.44
1:A:620:VAL:HG12	1:A:621:ASP:N	2.32	0.44
1:A:655:THR:HA	1:A:683:ARG:O	2.18	0.44
1:A:503:ALA:HB2	1:A:520:LEU:HD11	2.00	0.44
1:A:627:VAL:HG13	1:A:629:LEU:CD1	2.47	0.44
1:A:598:TYR:OH	2:X:8:DT:OP1	2.22	0.44
1:B:228:VAL:O	1:B:232:GLN:HG3	2.17	0.44
1:A:643:LEU:HD21	1:A:647[B]:ARG:CB	2.47	0.44
1:B:185:LEU:O	1:B:189:GLU:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:LYS:HD3	1:B:643:LEU:HD11	1.99	0.44
1:B:625:ASN:C	1:B:625:ASN:ND2	2.72	0.44
1:B:628:GLU:C	1:B:629:LEU:HD12	2.39	0.44
1:A:321:ALA:HA	1:A:326:ASN:O	2.18	0.43
1:A:631:GLY:O	1:A:634:LEU:HB2	2.19	0.43
1:B:398:GLY:O	1:B:401:THR:HG22	2.18	0.43
1:B:627:VAL:HG13	1:B:629:LEU:CD1	2.48	0.43
1:B:671:ASN:ND2	1:B:671:ASN:N	2.65	0.43
1:A:386:LEU:HB3	1:A:397:LEU:HD11	1.99	0.43
1:B:396:ARG:HG2	1:B:396:ARG:HH21	1.83	0.43
1:B:365:GLY:HA2	4:B:801:ANP:O1A	2.18	0.43
1:B:242:PHE:CE2	1:B:295:ARG:HD2	2.53	0.43
1:B:370:THR:HG21	1:B:397:LEU:HD21	2.01	0.43
1:A:437:VAL:HG12	1:A:437:VAL:O	2.19	0.43
1:A:612:LYS:HG2	1:A:619:THR:CG2	2.45	0.43
1:B:201:ILE:N	1:B:201:ILE:HD13	2.34	0.43
1:B:220:PRO:O	1:B:224:THR:HG22	2.19	0.43
1:A:628:GLU:C	1:A:629:LEU:HD12	2.39	0.43
1:B:665:MET:CE	1:B:695:ILE:HD13	2.40	0.43
1:A:302:LEU:HD22	1:A:306:LYS:HD2	2.00	0.42
1:A:681:ARG:HH21	1:A:681:ARG:HG3	1.83	0.42
1:B:600:ASN:O	1:B:601:GLU:HB2	2.19	0.42
1:A:587:PRO:HB3	1:A:612:LYS:HA	2.01	0.42
1:B:494:GLN:H	1:B:494:GLN:NE2	2.17	0.42
1:A:185:LEU:O	1:A:189:GLU:HG3	2.19	0.42
1:B:647[A]:ARG:CD	2:Y:5:DT:OP1	2.65	0.42
1:A:625:ASN:ND2	1:A:625:ASN:C	2.72	0.42
1:B:346:VAL:HG21	1:B:358:LEU:HG	2.00	0.42
1:B:346:VAL:HG23	1:B:486:ILE:HG12	2.01	0.42
1:B:655:THR:HA	1:B:683:ARG:O	2.20	0.42
1:A:242:PHE:CE2	1:A:295:ARG:HD2	2.54	0.42
1:A:672:LEU:HD13	1:A:672:LEU:C	2.40	0.42
1:B:434:VAL:O	1:B:461:VAL:HG13	2.19	0.42
1:A:386:LEU:HB3	1:A:397:LEU:HD12	2.00	0.42
1:A:397:LEU:O	1:A:401:THR:HB	2.19	0.42
1:A:257:ARG:HH11	1:A:257:ARG:HB2	1.83	0.42
1:A:366:LYS:HG2	1:A:488:LEU:HD12	2.00	0.42
1:B:417:GLN:CA	1:B:417:GLN:NE2	2.83	0.42
1:A:378:GLU:CD	1:A:403:ARG:HH21	2.23	0.42
1:A:554:ARG:HG3	2:X:4:DT:OP1	2.20	0.42
1:A:575:GLU:H	1:A:575:GLU:CD	2.13	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:LYS:NZ	1:A:497:LYS:N	2.66	0.42
1:B:321:ALA:HA	1:B:326:ASN:O	2.19	0.42
1:B:437:VAL:HG12	1:B:437:VAL:O	2.19	0.42
4:A:801:ANP:H2'	4:A:801:ANP:H5'2	1.65	0.41
1:A:357:VAL:HB	1:A:485:THR:CG2	2.32	0.41
1:B:350:LEU:O	1:B:457:ARG:HD3	2.20	0.41
1:B:616:ALA:O	1:B:630:THR:HG22	2.20	0.41
1:B:305:GLU:OE2	1:B:707:ALA:HB3	2.19	0.41
1:B:302:LEU:HD22	1:B:306:LYS:HD2	2.02	0.41
1:A:647[A]:ARG:CD	2:X:5:DT:OP1	2.68	0.41
1:A:600:ASN:O	1:A:601:GLU:HB2	2.21	0.41
1:A:417:GLN:NE2	1:A:417:GLN:CA	2.83	0.41
1:A:398:GLY:O	1:A:401:THR:HG22	2.21	0.41
1:B:598:TYR:OH	2:Y:8:DT:OP1	2.21	0.41
1:A:346:VAL:HG23	1:A:486:ILE:HG12	2.03	0.41
1:A:396:ARG:HG2	1:A:396:ARG:HH21	1.85	0.41
1:A:661:HIS:H	1:A:664:HIS:CD2	2.31	0.41
1:B:564:ASN:HD22	1:B:641:TYR:HB2	1.84	0.41
1:A:346:VAL:HG21	1:A:358:LEU:HG	2.03	0.41
1:A:553:MET:HE2	1:A:663:ALA:O	2.20	0.41
1:A:493:ARG:CD	1:A:652:GLU:OE1	2.68	0.41
1:B:366:LYS:HG2	1:B:488:LEU:HD12	2.02	0.41
1:B:475:PRO:HG2	5:B:83:HOH:O	2.20	0.41
1:A:207:ASP:OD1	1:A:222:ARG:HD2	2.21	0.41
1:B:194:THR:O	1:B:194:THR:HG22	2.21	0.41
1:B:310:SER:O	1:B:314:THR:HG23	2.21	0.41
1:B:392:LYS:HB3	1:B:392:LYS:HE2	1.91	0.41
1:B:515:TRP:CE3	1:B:520:LEU:HD22	2.56	0.41
1:B:672:LEU:C	1:B:672:LEU:HD13	2.41	0.41
1:A:242:PHE:C	1:A:242:PHE:CD2	2.94	0.41
1:A:449:LEU:HA	1:A:449:LEU:HD23	1.84	0.41
1:B:540:GLU:HG2	1:B:540:GLU:O	2.21	0.41
1:B:655:THR:HG21	1:B:683:ARG:NH2	2.21	0.41
1:A:671:ASN:N	1:A:671:ASN:ND2	2.68	0.40
1:B:538:VAL:HG13	1:B:547:VAL:CG1	2.51	0.40
1:A:515:TRP:CE3	1:A:520:LEU:HD22	2.57	0.40
1:A:250:LYS:HE3	1:B:508:LEU:HD13	2.03	0.40
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.82	0.40
1:B:256:THR:CG2	1:B:257:ARG:H	2.28	0.40
1:B:567:LEU:HD12	1:B:567:LEU:HA	1.85	0.40
1:B:449:LEU:HD23	1:B:449:LEU:HA	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	512/574 (89%)	474 (93%)	30 (6%)	8 (2%)	11	19
1	B	512/574 (89%)	476 (93%)	28 (6%)	8 (2%)	11	19
All	All	1024/1148 (89%)	950 (93%)	58 (6%)	16 (2%)	11	19

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ARG
1	A	575	GLU
1	B	257	ARG
1	B	575	GLU
1	A	576	GLY
1	B	576	GLY
1	A	258	VAL
1	A	185	LEU
1	B	185	LEU
1	B	258	VAL
1	A	261	GLY
1	B	261	GLY
1	A	260	PRO
1	B	260	PRO
1	A	665	MET
1	B	215	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/435 (91%)	354 (89%)	42 (11%)	8	15
1	B	396/435 (91%)	355 (90%)	41 (10%)	8	15
All	All	792/870 (91%)	709 (90%)	83 (10%)	8	15

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ARG
1	A	197	GLU
1	A	201	ILE
1	A	233	LEU
1	A	236	THR
1	A	302	LEU
1	A	308	LEU
1	A	333	LYS
1	A	336	ARG
1	A	355	LEU
1	A	358	LEU
1	A	370	THR
1	A	376	LEU
1	A	396	ARG
1	A	401	THR
1	A	417	GLN
1	A	432	LEU
1	A	436	GLU
1	A	444	LEU
1	A	459	LEU
1	A	461	VAL
1	A	486	ILE
1	A	494	GLN
1	A	520	LEU
1	A	521	ASN
1	A	533	ARG
1	A	564	ASN
1	A	567	LEU
1	A	572	ASN
1	A	575	GLU
1	A	579	ARG
1	A	619	THR
1	A	623	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	625	ASN
1	A	637	LEU
1	A	643	LEU
1	A	655	THR
1	A	665	MET
1	A	671	ASN
1	A	672	LEU
1	A	700[A]	GLN
1	A	700[B]	GLN
1	B	187	ARG
1	B	197	GLU
1	B	201	ILE
1	B	233	LEU
1	B	236	THR
1	B	302	LEU
1	B	308	LEU
1	B	333	LYS
1	B	336	ARG
1	B	355	LEU
1	B	358	LEU
1	B	370	THR
1	B	376	LEU
1	B	396	ARG
1	B	417	GLN
1	B	432	LEU
1	B	436	GLU
1	B	444	LEU
1	B	459	LEU
1	B	461	VAL
1	B	486	ILE
1	B	494	GLN
1	B	520	LEU
1	B	521	ASN
1	B	533	ARG
1	B	564	ASN
1	B	567	LEU
1	B	572	ASN
1	B	575	GLU
1	B	579	ARG
1	B	619	THR
1	B	623	ASP
1	B	625	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	637	LEU
1	B	643	LEU
1	B	655	THR
1	B	665	MET
1	B	671	ASN
1	B	672	LEU
1	B	700[A]	GLN
1	B	700[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	262	GLN
1	A	326	ASN
1	A	409	HIS
1	A	417	GLN
1	A	466	GLN
1	A	490	GLN
1	A	494	GLN
1	A	502	GLN
1	A	521	ASN
1	A	564	ASN
1	A	568	GLN
1	A	572	ASN
1	A	593	GLN
1	A	600	ASN
1	A	625	ASN
1	A	636	ASN
1	A	638	GLN
1	A	671	ASN
1	A	705	ASN
1	B	211	GLN
1	B	262	GLN
1	B	326	ASN
1	B	409	HIS
1	B	417	GLN
1	B	466	GLN
1	B	490	GLN
1	B	494	GLN
1	B	502	GLN
1	B	521	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	564	ASN
1	B	568	GLN
1	B	572	ASN
1	B	593	GLN
1	B	600	ASN
1	B	625	ASN
1	B	636	ASN
1	B	638	GLN
1	B	671	ASN
1	B	705	ASN

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	801	3	29,33,33	1.17	3 (10%)	28,52,52	2.23	7 (25%)
4	ANP	B	801	3	29,33,33	1.18	4 (13%)	28,52,52	2.24	6 (21%)

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	801	3	-	0/13/38/38	0/3/3/3
4	ANP	B	801	3	-	0/13/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	ANP	PB-O2B	-3.03	1.48	1.56
4	B	801	ANP	PB-O2B	-2.99	1.48	1.56
4	A	801	ANP	PB-O1B	2.02	1.48	1.46
4	B	801	ANP	PB-O1B	2.05	1.48	1.46
4	B	801	ANP	PG-O1G	2.08	1.48	1.46
4	A	801	ANP	O4'-C1'	2.16	1.44	1.41
4	B	801	ANP	O4'-C1'	2.20	1.44	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	ANP	N3-C2-N1	-8.32	121.61	128.86
4	A	801	ANP	N3-C2-N1	-8.23	121.69	128.86
4	A	801	ANP	C5'-C4'-C3'	-3.81	100.76	115.29
4	B	801	ANP	C5'-C4'-C3'	-3.67	101.29	115.29
4	B	801	ANP	PA-O3A-PB	-3.25	120.90	132.38
4	A	801	ANP	PA-O3A-PB	-2.98	121.86	132.38
4	A	801	ANP	C2'-C3'-C4'	-2.85	97.07	102.62
4	B	801	ANP	C2'-C3'-C4'	-2.60	97.56	102.62
4	B	801	ANP	C4'-O4'-C1'	-2.56	107.04	109.77
4	A	801	ANP	C4'-O4'-C1'	-2.50	107.10	109.77
4	A	801	ANP	C4-C5-N7	-2.27	107.22	109.41
4	A	801	ANP	O2B-PB-O1B	3.91	118.00	109.87
4	B	801	ANP	O2B-PB-O1B	4.10	118.39	109.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	ANP	3	0
4	B	801	ANP	4	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	516/574 (89%)	0.50	36 (6%) 17 17	18, 39, 83, 112	2 (0%)
1	B	516/574 (89%)	0.45	42 (8%) 13 12	21, 41, 84, 115	2 (0%)
2	X	7/8 (87%)	-0.02	0 100 100	37, 40, 67, 85	0
2	Y	7/8 (87%)	0.08	0 100 100	37, 42, 71, 86	0
All	All	1046/1164 (89%)	0.47	78 (7%) 15 15	18, 40, 84, 115	4 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	199	GLU	6.8
1	B	184	ALA	6.5
1	A	188	LEU	6.5
1	B	195	LEU	6.4
1	B	194	THR	6.3
1	A	195	LEU	6.3
1	B	273	LEU	6.0
1	B	217	LEU	5.4
1	B	185	LEU	5.4
1	B	196	THR	5.4
1	B	210	TRP	5.2
1	A	196	THR	5.2
1	B	209	LEU	4.7
1	A	700[A]	GLN	4.7
1	B	190	LYS	4.6
1	B	187	ARG	4.5
1	B	188	LEU	4.5
1	B	700[A]	GLN	4.4
1	B	192	LEU	4.3
1	B	201	ILE	4.0
1	B	215	GLY	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	263	ALA	3.6
1	A	209	LEU	3.5
1	A	192	LEU	3.4
1	A	185	LEU	3.4
1	A	326	ASN	3.4
1	A	190	LYS	3.3
1	A	273	LEU	3.3
1	A	265	LEU	3.3
1	A	197	GLU	3.2
1	A	256	THR	3.2
1	B	193	PHE	3.2
1	A	260	PRO	3.1
1	B	262	GLN	3.1
1	B	265	LEU	3.0
1	B	258	VAL	3.0
1	B	647[A]	ARG	3.0
1	B	208	LYS	3.0
1	A	194	THR	2.9
1	A	258	VAL	2.9
1	A	184	ALA	2.9
1	A	647[A]	ARG	2.8
1	A	200	GLY	2.8
1	A	575	GLU	2.8
1	B	206	ALA	2.8
1	B	256	THR	2.7
1	B	212	ALA	2.7
1	A	278	GLU	2.7
1	A	203	PHE	2.7
1	B	223	LEU	2.7
1	B	255	TYR	2.6
1	A	257	ARG	2.6
1	B	197	GLU	2.6
1	B	198	VAL	2.5
1	B	191	ASP	2.5
1	A	212	ALA	2.5
1	A	223	LEU	2.4
1	B	269	THR	2.4
1	A	191	ASP	2.4
1	A	210	TRP	2.4
1	A	271	VAL	2.4
1	B	257	ARG	2.3
1	A	225	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	272	GLU	2.3
1	B	260	PRO	2.3
1	A	269	THR	2.2
1	B	211	GLN	2.2
1	B	575	GLU	2.2
1	B	266	ALA	2.2
1	B	714	ALA	2.2
1	B	322	ASP	2.2
1	B	213	ARG	2.2
1	B	414	TYR	2.2
1	A	255	TYR	2.1
1	A	245	ARG	2.1
1	A	201	ILE	2.0
1	B	614	GLU	2.0
1	A	328	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ANP	A	801	31/31	0.96	0.19	0.36	14,33,46,61	0
4	ANP	B	801	31/31	0.97	0.14	-0.47	22,35,47,56	0
3	MG	A	800	1/1	0.95	0.13	-	21,21,21,21	0
3	MG	B	800	1/1	0.98	0.06	-	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.