



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:39 PM GMT

PDB ID : 2ONJ  
Title : Structure of the multidrug ABC transporter Sav1866 from *S. aureus* in complex with AMP-PNP  
Authors : Dawson, R.J.P.; Locher, K.P.  
Deposited on : 2007-01-24  
Resolution : 3.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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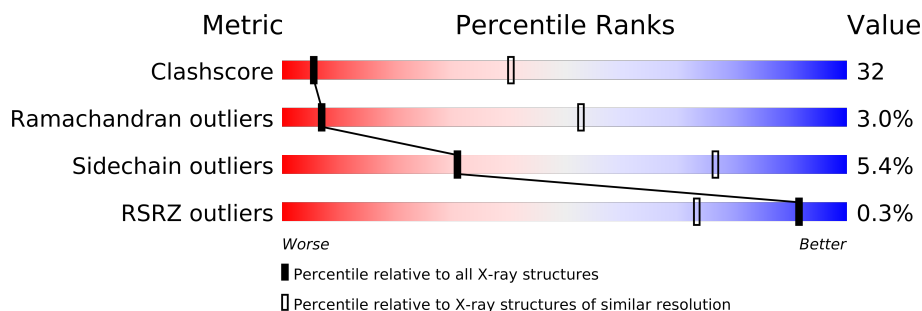
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.40 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))
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	578	
1	B	578	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9254 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

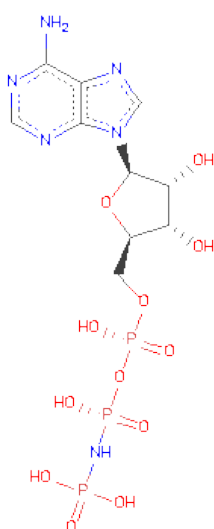
- Molecule 1 is a protein called Multidrug export ATP-binding/permease protein SAV1866.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4584	2967	774	834	9			
1	B	578	Total	C	N	O	S	0	0	0
			4584	2967	774	834	9			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Na	0	0
			2	2		
2	A	2	Total	Na	0	0
			2	2		

- Molecule 3 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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

- Molecule 4 is water.

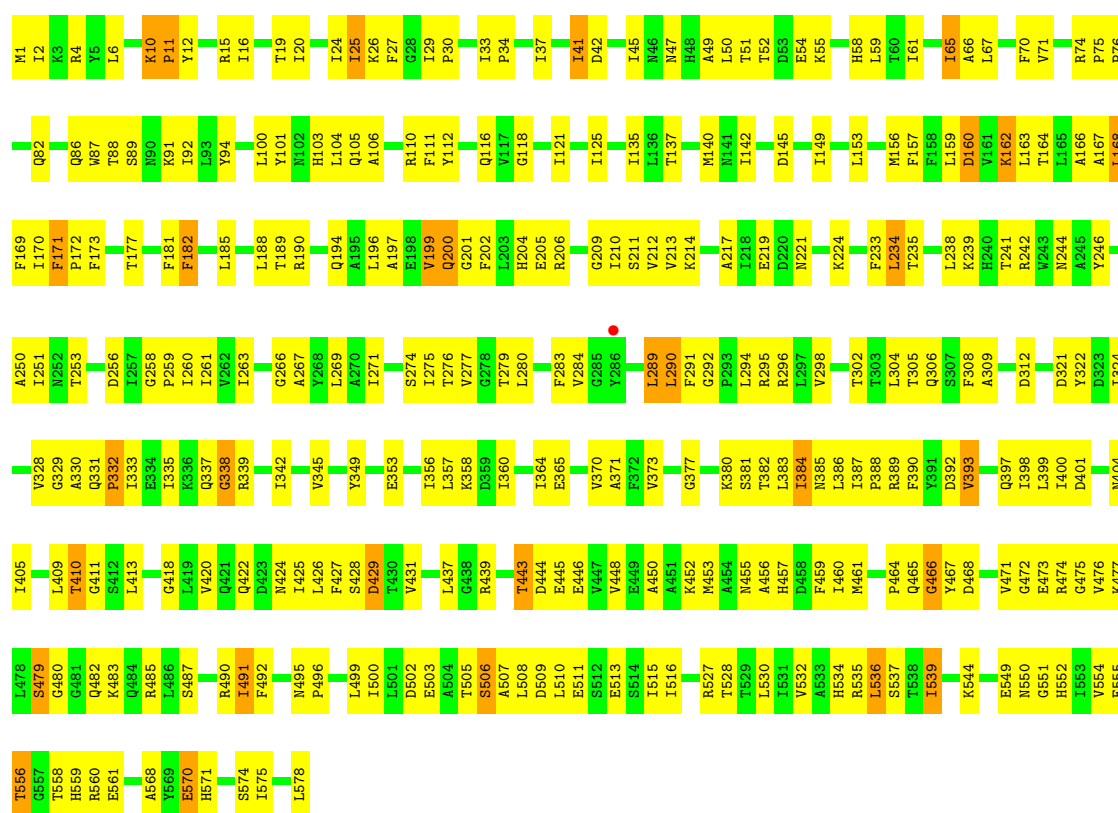
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	10	Total	O	0	0
			10	10		

### 3 Residue-property plots

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.

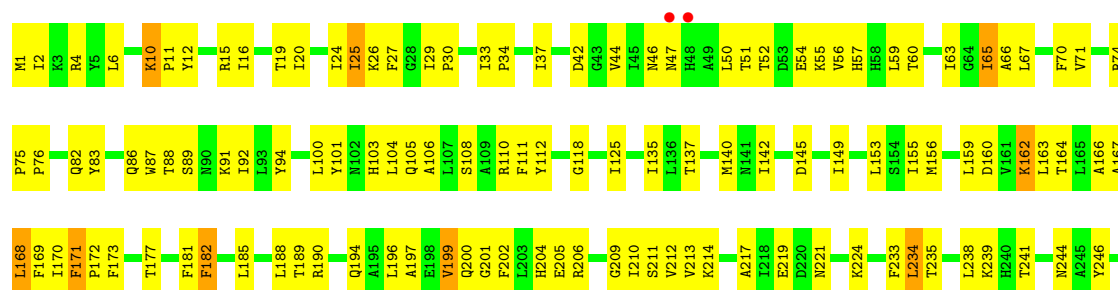
- Molecule 1: Multidrug export ATP-binding/permease protein SAV1866

Chain A:



- Molecule 1: Multidrug export ATP-binding/permease protein SAV1866

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.96Å 104.45Å 181.39Å 90.00° 98.23° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 29.59 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.40) 99.9 (29.59-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 3.39Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.254 , 0.278 0.255 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	101.1	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 87.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 41082 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.42	0/4669	0.66	1/6328 (0.0%)
1	B	0.42	0/4669	0.67	1/6328 (0.0%)
All	All	0.42	0/9338	0.67	2/12656 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	LEU	CA-CB-CG	6.64	130.56	115.30
1	A	234	LEU	CB-CG-CD1	-5.28	102.03	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4584	0	4713	327	0
1	B	4584	0	4714	332	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	12	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	12	9	0
4	A	10	0	0	3	0
4	B	10	0	0	3	0
All	All	9254	0	9451	598	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

All (598) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:15:ARG:HD2	1:A:15:ARG:H	1.05	1.19
1:A:52:THR:HA	1:A:55:LYS:HE2	1.18	1.17
1:A:94:TYR:CD1	1:B:234:LEU:HD21	1.79	1.16
1:A:234:LEU:HD21	1:B:94:TYR:CD1	1.84	1.13
1:A:94:TYR:CD1	1:B:234:LEU:CD2	2.36	1.08
1:B:15:ARG:H	1:B:15:ARG:HD2	1.05	1.07
1:A:234:LEU:CD2	1:B:94:TYR:CD1	2.38	1.07
1:B:276:THR:HG22	1:B:278:GLY:H	1.23	1.02
1:B:44:VAL:HG13	1:B:55:LYS:HB2	1.42	1.01
1:A:94:TYR:CG	1:B:234:LEU:HD21	1.95	1.00
1:B:156:MET:HB3	1:B:164:THR:HG22	1.45	0.98
1:A:234:LEU:HD21	1:B:94:TYR:CG	2.00	0.95
1:A:234:LEU:HD21	1:B:94:TYR:HB2	1.48	0.93
1:A:276:THR:HG22	1:A:277:VAL:H	1.31	0.92
1:A:263:ILE:HG22	1:B:63:ILE:HD11	1.50	0.91
1:A:75:PRO:HB2	1:A:76:PRO:HD3	1.52	0.91
1:A:505:THR:HG21	1:A:513:GLU:OE2	1.70	0.91
1:B:505:THR:HG21	1:B:513:GLU:OE2	1.71	0.91
1:A:335:ILE:HD13	1:A:400:ILE:HG21	1.54	0.90
1:A:15:ARG:N	1:A:15:ARG:HD2	1.87	0.89
1:B:75:PRO:HB2	1:B:76:PRO:HD3	1.53	0.88
1:B:335:ILE:HD13	1:B:400:ILE:HG21	1.54	0.88
1:A:234:LEU:HD21	1:B:94:TYR:CB	2.04	0.87
1:B:15:ARG:N	1:B:15:ARG:HD2	1.87	0.86
1:B:51:THR:HB	1:B:54:GLU:HG2	1.59	0.84
1:A:455:ASN:HD22	1:A:515:ILE:HG21	1.42	0.84
1:B:455:ASN:HD22	1:B:515:ILE:HG21	1.43	0.83
1:A:204:HIS:HD2	1:B:204:HIS:ND1	1.77	0.82
1:A:558:THR:HB	1:A:561:GLU:HG3	1.62	0.82
1:A:162:LYS:H	1:A:162:LYS:HD3	1.44	0.81
1:A:234:LEU:HD23	1:B:94:TYR:CD1	2.15	0.81
1:B:428:SER:HB2	1:B:473:GLU:HA	1.65	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:275:ILE:HG22	1:A:276:THR:H	1.47	0.79
1:B:558:THR:HB	1:B:561:GLU:HG3	1.62	0.79
1:A:94:TYR:HB2	1:B:234:LEU:HD21	1.63	0.79
1:B:209:GLY:O	1:B:212:VAL:HG12	1.84	0.78
1:B:331:GLN:O	1:B:333:ILE:HG13	1.83	0.78
1:A:234:LEU:CD2	1:B:94:TYR:HD1	1.96	0.78
1:A:94:TYR:CB	1:B:234:LEU:HD21	2.13	0.77
1:A:331:GLN:O	1:A:333:ILE:HG13	1.84	0.77
1:A:353:GLU:HG2	1:B:464:PRO:HG3	1.65	0.77
1:A:397:GLN:HE21	1:A:399:LEU:HD11	1.50	0.76
1:B:397:GLN:HE21	1:B:399:LEU:HD11	1.50	0.76
1:A:364:ILE:HD13	1:A:530:LEU:HD21	1.68	0.76
1:A:209:GLY:O	1:A:212:VAL:HG12	1.85	0.76
1:A:142:ILE:HD11	1:A:304:LEU:HD11	1.67	0.76
1:B:332:PRO:HD3	1:B:409:LEU:HD12	1.67	0.76
1:B:364:ILE:HD13	1:B:530:LEU:HD21	1.67	0.76
1:A:332:PRO:HD3	1:A:409:LEU:HD12	1.68	0.75
1:B:142:ILE:HD11	1:B:304:LEU:HD11	1.68	0.75
1:B:162:LYS:H	1:B:162:LYS:HD3	1.52	0.75
1:B:276:THR:HG22	1:B:278:GLY:N	2.00	0.74
1:B:381:SER:OG	4:B:808:HOH:O	2.06	0.74
1:A:428:SER:HB2	1:A:473:GLU:HA	1.68	0.74
1:B:410:THR:HG22	1:B:411:GLY:N	2.02	0.73
1:A:94:TYR:HD1	1:B:234:LEU:CD2	2.02	0.73
1:A:410:THR:HG22	1:A:411:GLY:N	2.03	0.73
1:B:534:HIS:O	1:B:536:LEU:HD23	1.88	0.72
1:A:534:HIS:O	1:A:536:LEU:HD23	1.89	0.72
1:A:387:ILE:C	1:A:389:ARG:H	1.93	0.72
1:B:262:VAL:HG11	1:B:287:LEU:HD21	1.71	0.72
1:A:204:HIS:CD2	1:B:204:HIS:ND1	2.57	0.72
1:A:160:ASP:O	1:A:164:THR:HG23	1.90	0.71
1:B:459:PHE:CE1	1:B:482:GLN:HG2	2.24	0.71
1:A:473:GLU:O	1:A:476:VAL:HG23	1.90	0.71
1:B:387:ILE:HB	1:B:388:PRO:HD3	1.73	0.71
1:A:94:TYR:CD1	1:B:234:LEU:HD23	2.24	0.71
1:B:387:ILE:C	1:B:389:ARG:H	1.92	0.70
1:A:387:ILE:HB	1:A:388:PRO:HD3	1.73	0.70
1:A:459:PHE:CE1	1:A:482:GLN:HG2	2.26	0.70
1:B:356:ILE:CD1	3:B:700:ANP:H1'	2.22	0.69
1:B:473:GLU:O	1:B:476:VAL:HG23	1.92	0.69
1:B:431:VAL:HG11	1:B:460:ILE:HD13	1.75	0.68
1:A:338:GLY:HA3	1:A:528:THR:OG1	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:338:GLY:HA3	1:B:528:THR:OG1	1.92	0.68
1:A:276:THR:HG22	1:A:277:VAL:N	2.07	0.68
1:B:42:ASP:HA	1:B:46:ASN:HB2	1.74	0.67
1:A:52:THR:CA	1:A:55:LYS:HE2	2.10	0.67
1:A:47:ASN:HD22	1:A:50:LEU:HG	1.58	0.67
1:A:330:ALA:O	1:A:331:GLN:HG2	1.96	0.66
1:B:51:THR:CB	1:B:54:GLU:HG2	2.25	0.66
1:B:258:GLY:HA3	1:B:291:PHE:CE2	2.31	0.66
1:A:106:ALA:HB3	1:A:322:TYR:HE2	1.61	0.66
1:A:116:GLN:HA	1:B:473:GLU:OE1	1.96	0.66
1:A:258:GLY:HA3	1:A:291:PHE:CE2	2.31	0.65
1:B:25:ILE:HG22	1:B:25:ILE:O	1.96	0.65
1:B:106:ALA:HB3	1:B:322:TYR:HE2	1.61	0.65
1:A:37:ILE:CG1	1:B:263:ILE:HD11	2.27	0.65
1:A:464:PRO:HG3	1:B:353:GLU:HG2	1.79	0.65
1:A:431:VAL:HG11	1:A:460:ILE:HD13	1.77	0.64
1:A:25:ILE:O	1:A:25:ILE:HG22	1.96	0.64
1:A:384:ILE:HD12	1:A:532:VAL:CG2	2.27	0.64
1:A:15:ARG:CD	1:A:15:ARG:H	1.95	0.64
1:B:15:ARG:H	1:B:15:ARG:CD	1.95	0.64
1:B:384:ILE:HD12	1:B:532:VAL:CG2	2.28	0.64
1:A:275:ILE:HG22	1:A:276:THR:N	2.13	0.64
1:B:330:ALA:O	1:B:331:GLN:HG2	1.97	0.64
1:A:37:ILE:HG12	1:B:263:ILE:HD11	1.80	0.64
1:B:472:GLY:O	1:B:475:GLY:N	2.31	0.64
1:B:491:ILE:HD13	1:B:499:LEU:HD22	1.79	0.64
1:B:160:ASP:OD2	1:B:163:LEU:HB2	1.97	0.64
1:B:485:ARG:HG2	1:B:516:ILE:HD11	1.80	0.63
1:A:170:ILE:HG13	1:A:258:GLY:HA2	1.80	0.63
1:B:549:GLU:HB2	1:B:554:VAL:HG21	1.79	0.63
1:A:549:GLU:HB2	1:A:554:VAL:HG21	1.79	0.63
1:A:118:GLY:HA3	1:A:201:GLY:HA2	1.80	0.63
1:B:162:LYS:HE2	1:B:275:ILE:HD11	1.80	0.63
1:A:485:ARG:HG2	1:A:516:ILE:HD11	1.80	0.63
1:A:472:GLY:O	1:A:475:GLY:N	2.31	0.62
1:B:118:GLY:HA3	1:B:201:GLY:HA2	1.80	0.62
1:A:337:GLN:O	1:A:401:ASP:OD2	2.17	0.62
1:B:506:SER:O	1:B:535:ARG:NH2	2.32	0.62
1:B:170:ILE:HG13	1:B:258:GLY:HA2	1.80	0.62
1:A:506:SER:O	1:A:535:ARG:NH2	2.32	0.62
1:A:491:ILE:HD13	1:A:499:LEU:HD22	1.80	0.62
1:A:256:ASP:HB3	1:B:70:PHE:HD2	1.64	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:450:ALA:O	1:A:453:MET:HB2	2.00	0.62
1:B:358:LYS:HD2	1:B:552:HIS:NE2	2.14	0.62
1:A:495:ASN:CG	1:A:527:ARG:HH22	2.03	0.61
1:A:202:PHE:CE2	1:A:206:ARG:HG3	2.35	0.61
1:A:269:LEU:HB3	1:A:274:SER:CB	2.30	0.61
1:B:357:LEU:HD22	1:B:360:ILE:HD11	1.83	0.61
1:B:337:GLN:O	1:B:401:ASP:OD2	2.18	0.61
1:B:495:ASN:CG	1:B:527:ARG:HH22	2.03	0.61
1:B:450:ALA:O	1:B:453:MET:HB2	2.00	0.61
1:A:387:ILE:C	1:A:389:ARG:N	2.54	0.61
1:A:455:ASN:ND2	1:A:515:ILE:HG21	2.14	0.61
1:B:185:LEU:HB2	1:B:305:THR:HG21	1.82	0.61
1:A:381:SER:CB	4:A:818:HOH:O	2.48	0.61
1:A:185:LEU:HB2	1:A:305:THR:HG21	1.82	0.60
1:A:377:GLY:C	3:A:701:ANP:O1A	2.40	0.60
1:A:70:PHE:HD2	1:B:256:ASP:HB3	1.66	0.60
1:B:202:PHE:CE2	1:B:206:ARG:HG3	2.35	0.60
1:A:358:LYS:HD2	1:A:552:HIS:NE2	2.15	0.60
1:A:357:LEU:HD22	1:A:360:ILE:HD11	1.83	0.60
1:B:387:ILE:C	1:B:389:ARG:N	2.53	0.60
1:B:405:ILE:HG23	1:B:413:LEU:HD21	1.84	0.60
1:B:455:ASN:ND2	1:B:515:ILE:HG21	2.15	0.60
1:B:425:ILE:O	1:B:426:LEU:HD23	2.02	0.59
1:A:558:THR:HG22	1:A:560:ARG:H	1.68	0.59
1:A:425:ILE:O	1:A:426:LEU:HD23	2.02	0.59
1:B:106:ALA:CB	1:B:322:TYR:HE2	2.15	0.59
1:B:443:THR:HB	1:B:446:GLU:HG3	1.84	0.59
1:A:405:ILE:HG23	1:A:413:LEU:HD21	1.84	0.59
1:B:181:PHE:O	1:B:182:PHE:C	2.42	0.59
1:A:71:VAL:O	1:A:71:VAL:HG12	2.02	0.59
1:A:536:LEU:H	1:A:536:LEU:HD23	1.68	0.58
1:B:71:VAL:O	1:B:71:VAL:HG12	2.01	0.58
1:A:349:TYR:HE1	1:A:356:ILE:HD12	1.68	0.58
1:A:217:ALA:HA	1:A:219:GLU:OE1	2.03	0.58
1:A:574:SER:O	1:A:578:LEU:HB2	2.03	0.58
1:B:558:THR:HG22	1:B:560:ARG:H	1.67	0.58
1:A:398:ILE:HB	1:A:405:ILE:HD12	1.86	0.58
1:A:47:ASN:HD22	1:A:50:LEU:CG	2.17	0.58
1:B:405:ILE:HG23	1:B:413:LEU:CD2	2.34	0.58
1:A:106:ALA:CB	1:A:322:TYR:HE2	2.15	0.58
1:B:210:ILE:O	1:B:211:SER:C	2.41	0.58
1:B:387:ILE:O	1:B:389:ARG:N	2.36	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:398:ILE:HB	1:B:405:ILE:HD12	1.85	0.58
1:A:443:THR:HB	1:A:446:GLU:HG3	1.84	0.58
1:A:387:ILE:O	1:A:389:ARG:N	2.37	0.57
1:B:217:ALA:HA	1:B:219:GLU:OE1	2.03	0.57
1:B:356:ILE:HD12	3:B:700:ANP:H1'	1.86	0.57
1:A:399:LEU:HD23	1:A:404:ASN:HA	1.87	0.57
1:B:267:ALA:C	1:B:269:LEU:H	2.07	0.57
1:A:405:ILE:HG23	1:A:413:LEU:CD2	2.35	0.57
1:A:418:GLY:HA3	1:A:496:PRO:HG3	1.87	0.57
1:B:137:THR:O	1:B:142:ILE:HG13	2.03	0.57
1:B:384:ILE:HG22	1:B:385:ASN:N	2.20	0.57
1:A:137:THR:O	1:A:142:ILE:HG13	2.04	0.57
1:A:181:PHE:O	1:A:182:PHE:C	2.42	0.57
1:B:536:LEU:HD23	1:B:536:LEU:H	1.68	0.57
1:B:56:VAL:O	1:B:56:VAL:HG12	2.05	0.56
1:B:371:ALA:CB	1:B:539:ILE:HG13	2.35	0.56
1:B:444:ASP:O	1:B:448:VAL:HG23	2.05	0.56
1:B:275:ILE:HG22	1:B:276:THR:N	2.20	0.56
1:B:349:TYR:HE1	1:B:356:ILE:HD12	1.70	0.56
1:A:453:MET:HB3	1:A:492:PHE:CE2	2.40	0.56
1:B:418:GLY:HA3	1:B:496:PRO:HG3	1.87	0.56
1:A:371:ALA:CB	1:A:539:ILE:HG13	2.35	0.56
1:B:63:ILE:O	1:B:63:ILE:HG22	2.05	0.56
1:B:453:MET:HB3	1:B:492:PHE:CE2	2.41	0.56
1:A:309:ALA:O	1:A:312:ASP:HB2	2.05	0.56
1:B:19:THR:HG21	1:B:140:MET:HE3	1.88	0.56
1:A:384:ILE:HD13	1:A:500:ILE:CG2	2.36	0.56
1:A:260:ILE:HG21	1:B:67:LEU:HD21	1.86	0.56
1:A:384:ILE:HG22	1:A:385:ASN:N	2.21	0.56
1:A:444:ASP:O	1:A:448:VAL:HG23	2.04	0.56
1:B:399:LEU:HD23	1:B:404:ASN:HA	1.87	0.56
1:A:491:ILE:HG22	1:A:492:PHE:N	2.21	0.56
1:B:155:ILE:HG21	1:B:286:TYR:CE2	2.41	0.56
1:B:384:ILE:HD13	1:B:500:ILE:CG2	2.36	0.56
1:B:309:ALA:O	1:B:312:ASP:HB2	2.05	0.56
1:B:47:ASN:HD22	1:B:50:LEU:HD21	1.71	0.55
1:A:26:LYS:O	1:A:30:PRO:HD2	2.06	0.55
1:A:345:VAL:HG13	1:A:393:VAL:CG2	2.35	0.55
1:A:162:LYS:N	1:A:162:LYS:HD3	2.18	0.55
1:A:269:LEU:HB3	1:A:274:SER:HB3	1.89	0.55
1:B:345:VAL:HG13	1:B:393:VAL:CG2	2.36	0.55
1:A:156:MET:HB3	1:A:283:PHE:CE1	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:16:ILE:O	1:B:20:ILE:HG13	2.06	0.55
1:A:92:ILE:HD12	1:A:135:ILE:HD13	1.89	0.55
1:A:177:THR:HB	1:A:251:ILE:HD13	1.89	0.55
1:B:177:THR:HB	1:B:251:ILE:HD13	1.88	0.55
1:A:276:THR:CG2	1:A:277:VAL:H	2.12	0.55
1:A:210:ILE:HG22	1:A:214:LYS:HG2	1.88	0.55
1:B:60:THR:O	1:B:60:THR:HG22	2.07	0.55
1:B:357:LEU:HB3	1:B:360:ILE:HD11	1.89	0.55
1:A:210:ILE:O	1:A:211:SER:C	2.43	0.55
1:A:16:ILE:O	1:A:20:ILE:HG13	2.07	0.55
1:A:206:ARG:NH1	1:B:427:PHE:CE1	2.76	0.55
1:A:479:SER:OG	1:A:480:GLY:N	2.40	0.55
1:A:75:PRO:HB2	1:A:76:PRO:CD	2.34	0.54
1:B:142:ILE:CD1	1:B:304:LEU:HD11	2.37	0.54
1:B:26:LYS:O	1:B:30:PRO:HD2	2.06	0.54
1:A:19:THR:HG21	1:A:140:MET:HE3	1.89	0.54
1:B:52:THR:O	1:B:52:THR:HG22	2.08	0.54
1:B:210:ILE:HG22	1:B:214:LYS:HG2	1.88	0.54
1:A:389:ARG:HD2	1:A:405:ILE:HG22	1.89	0.54
1:A:159:LEU:HD23	1:A:283:PHE:HD1	1.73	0.54
1:B:491:ILE:HG22	1:B:492:PHE:N	2.21	0.54
1:A:142:ILE:CD1	1:A:304:LEU:HD11	2.36	0.54
1:B:24:ILE:C	1:B:26:LYS:H	2.11	0.54
1:A:536:LEU:HD23	1:A:536:LEU:N	2.23	0.54
1:B:92:ILE:HD12	1:B:135:ILE:HD13	1.90	0.54
1:B:389:ARG:HD2	1:B:405:ILE:HG22	1.89	0.54
1:A:156:MET:HB3	1:A:164:THR:HG22	1.88	0.54
1:A:479:SER:HB2	3:B:700:ANP:O3A	2.08	0.54
1:B:277:VAL:O	1:B:277:VAL:HG12	2.08	0.54
1:A:12:TYR:HA	1:A:15:ARG:HD3	1.89	0.54
1:A:353:GLU:CG	1:B:464:PRO:HG3	2.36	0.54
1:B:549:GLU:HB2	1:B:554:VAL:CG2	2.38	0.53
1:A:2:ILE:HD11	1:A:308:PHE:HE2	1.72	0.53
1:A:157:PHE:HA	1:A:164:THR:HG21	1.90	0.53
1:B:12:TYR:HA	1:B:15:ARG:HD3	1.90	0.53
1:B:357:LEU:HB3	1:B:360:ILE:CD1	2.38	0.53
1:B:156:MET:HB3	1:B:164:THR:CG2	2.30	0.53
1:B:160:ASP:O	1:B:164:THR:HG23	2.08	0.53
1:B:2:ILE:HD11	1:B:308:PHE:HE2	1.73	0.53
1:B:479:SER:OG	1:B:480:GLY:N	2.40	0.53
1:A:24:ILE:C	1:A:26:LYS:H	2.11	0.53
1:B:536:LEU:HD23	1:B:536:LEU:N	2.23	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:LEU:HD21	1:B:260:ILE:HG21	1.89	0.52
1:A:357:LEU:HB3	1:A:360:ILE:CD1	2.39	0.52
1:A:357:LEU:HB3	1:A:360:ILE:HD11	1.91	0.52
1:A:464:PRO:HB2	1:A:465:GLN:NE2	2.24	0.52
1:A:549:GLU:HB2	1:A:554:VAL:CG2	2.39	0.52
1:B:324:ILE:HD11	1:B:390:PHE:C	2.30	0.52
1:A:345:VAL:HG13	1:A:393:VAL:HG23	1.91	0.52
1:A:159:LEU:O	1:A:160:ASP:HB2	2.10	0.52
1:A:335:ILE:CD1	1:A:400:ILE:HG21	2.35	0.52
1:A:324:ILE:HD11	1:A:390:PHE:C	2.31	0.52
1:A:33:ILE:HB	1:A:34:PRO:CD	2.40	0.52
1:B:33:ILE:HB	1:B:34:PRO:CD	2.40	0.52
1:A:349:TYR:CE1	1:A:356:ILE:HD12	2.44	0.52
1:A:495:ASN:ND2	1:A:527:ARG:HH22	2.08	0.52
1:A:41:ILE:HG22	1:A:42:ASP:N	2.24	0.52
1:A:234:LEU:CD2	1:B:94:TYR:HB2	2.29	0.51
1:B:163:LEU:HD23	1:B:283:PHE:CG	2.46	0.51
1:B:459:PHE:CZ	1:B:482:GLN:HG2	2.45	0.51
1:B:335:ILE:CD1	1:B:400:ILE:HG21	2.35	0.51
1:A:65:ILE:HG22	1:A:66:ALA:N	2.25	0.51
1:A:337:GLN:O	1:A:339:ARG:N	2.43	0.51
1:B:337:GLN:O	1:B:339:ARG:N	2.43	0.51
1:B:495:ASN:ND2	1:B:527:ARG:HH22	2.08	0.51
1:B:196:LEU:HB2	1:B:233:PHE:CE1	2.44	0.51
1:A:209:GLY:HA2	1:B:425:ILE:HD13	1.92	0.51
1:A:196:LEU:HB2	1:A:233:PHE:CE1	2.45	0.51
1:B:464:PRO:HB2	1:B:465:GLN:NE2	2.26	0.51
1:A:418:GLY:CA	1:A:496:PRO:HG3	2.41	0.51
1:B:461:MET:CE	1:B:461:MET:HA	2.41	0.51
3:A:701:ANP:O3A	1:B:479:SER:HB2	2.10	0.51
1:B:345:VAL:HG13	1:B:393:VAL:HG23	1.92	0.51
1:A:173:PHE:HD1	1:A:173:PHE:H	1.59	0.51
1:A:459:PHE:CZ	1:A:482:GLN:HG2	2.45	0.51
1:B:92:ILE:CD1	1:B:135:ILE:HD13	2.41	0.51
1:A:200:GLN:HG2	1:B:125:ILE:CD1	2.41	0.51
1:A:304:LEU:O	1:A:308:PHE:HD1	1.94	0.51
1:B:349:TYR:CE1	1:B:356:ILE:HD12	2.46	0.51
1:B:328:VAL:HG23	1:B:329:GLY:N	2.26	0.50
1:A:328:VAL:HG23	1:A:329:GLY:N	2.26	0.50
1:A:364:ILE:HD13	1:A:530:LEU:CD2	2.40	0.50
1:B:575:ILE:O	1:B:575:ILE:HG22	2.10	0.50
1:A:427:PHE:CE1	1:B:206:ARG:NH1	2.79	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:364:ILE:HD13	1:B:530:LEU:CD2	2.39	0.50
1:A:356:ILE:CD1	3:A:701:ANP:H1'	2.42	0.50
1:A:92:ILE:CD1	1:A:135:ILE:HD13	2.41	0.50
1:A:125:ILE:CD1	1:B:200:GLN:HG2	2.40	0.50
1:A:575:ILE:HG22	1:A:575:ILE:O	2.11	0.50
1:A:153:LEU:HD11	1:A:168:LEU:HD21	1.94	0.50
1:A:177:THR:CG2	1:A:251:ILE:HD13	2.42	0.50
1:B:177:THR:CG2	1:B:251:ILE:HD13	2.42	0.50
1:B:65:ILE:HG22	1:B:66:ALA:N	2.26	0.50
1:A:384:ILE:HD12	1:A:532:VAL:HG23	1.94	0.50
1:B:418:GLY:CA	1:B:496:PRO:HG3	2.42	0.50
1:B:173:PHE:H	1:B:173:PHE:HD1	1.58	0.50
1:A:1:MET:O	1:A:4:ARG:HB2	2.12	0.50
1:B:75:PRO:HB2	1:B:76:PRO:CD	2.35	0.50
1:B:342:ILE:HG23	1:B:345:VAL:HG21	1.94	0.50
1:A:153:LEU:HD21	1:A:168:LEU:HD21	1.93	0.50
1:A:94:TYR:HB2	1:B:234:LEU:CD2	2.37	0.50
1:A:473:GLU:C	1:A:475:GLY:H	2.14	0.50
1:A:260:ILE:HG21	1:B:67:LEU:CD2	2.42	0.49
1:B:384:ILE:HD12	1:B:532:VAL:HG23	1.94	0.49
1:A:456:ALA:O	1:A:457:HIS:C	2.51	0.49
1:B:153:LEU:HD11	1:B:168:LEU:HD21	1.95	0.49
1:B:379:GLY:N	3:B:700:ANP:O1A	2.46	0.49
1:A:269:LEU:HB3	1:A:274:SER:OG	2.11	0.49
1:A:45:ILE:HG21	1:B:277:VAL:HG11	1.95	0.49
1:B:153:LEU:HD21	1:B:168:LEU:HD21	1.93	0.49
1:A:51:THR:HB	1:A:54:GLU:HG2	1.94	0.49
1:A:461:MET:HA	1:A:461:MET:CE	2.42	0.49
1:B:212:VAL:HG13	1:B:213:VAL:N	2.27	0.49
1:B:1:MET:O	1:B:4:ARG:HB2	2.12	0.49
1:A:47:ASN:ND2	1:A:50:LEU:HG	2.27	0.49
1:B:91:LYS:O	1:B:94:TYR:HB3	2.13	0.49
1:B:304:LEU:O	1:B:308:PHE:HD1	1.94	0.49
1:B:456:ALA:O	1:B:457:HIS:C	2.51	0.48
1:A:167:ALA:O	1:A:169:PHE:N	2.46	0.48
1:B:74:ARG:HB3	1:B:75:PRO:HD3	1.95	0.48
1:A:106:ALA:CB	1:A:322:TYR:CE2	2.96	0.48
1:A:443:THR:HG22	1:A:445:GLU:OE1	2.14	0.48
1:A:428:SER:N	1:B:205:GLU:OE1	2.41	0.48
1:B:377:GLY:C	3:B:700:ANP:O1A	2.52	0.48
1:B:106:ALA:O	1:B:322:TYR:HD2	1.96	0.48
1:B:101:TYR:OH	1:B:105:GLN:NE2	2.46	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:91:LYS:O	1:A:94:TYR:HB3	2.13	0.48
1:A:342:ILE:HG23	1:A:345:VAL:HG21	1.94	0.48
1:B:473:GLU:C	1:B:475:GLY:H	2.17	0.48
1:B:89:SER:HA	1:B:92:ILE:HD12	1.95	0.48
1:B:171:PHE:CE1	1:B:294:LEU:HD11	2.49	0.48
1:A:145:ASP:O	1:A:149:ILE:HG13	2.14	0.48
1:B:381:SER:CB	4:B:808:HOH:O	2.59	0.48
1:B:106:ALA:CB	1:B:322:TYR:CE2	2.96	0.48
1:A:74:ARG:HB3	1:A:75:PRO:HD3	1.96	0.48
1:B:260:ILE:C	1:B:262:VAL:H	2.17	0.48
1:B:544:LYS:HE3	1:B:556:THR:HG23	1.96	0.48
1:A:212:VAL:HG13	1:A:213:VAL:N	2.27	0.47
1:B:145:ASP:O	1:B:149:ILE:HG13	2.14	0.47
1:A:106:ALA:O	1:A:322:TYR:HD2	1.97	0.47
1:B:47:ASN:ND2	1:B:50:LEU:HD21	2.29	0.47
1:A:89:SER:HA	1:A:92:ILE:HD12	1.95	0.47
1:A:125:ILE:HD13	1:B:200:GLN:HG2	1.96	0.47
1:A:163:LEU:HG	1:A:283:PHE:CE2	2.50	0.47
1:A:479:SER:OG	3:B:700:ANP:N3B	2.47	0.47
1:A:101:TYR:OH	1:A:105:GLN:NE2	2.46	0.47
1:A:544:LYS:HE3	1:A:556:THR:HG23	1.96	0.47
1:A:171:PHE:CE1	1:A:294:LEU:HD11	2.49	0.47
1:B:443:THR:HG22	1:B:445:GLU:OE1	2.14	0.47
1:A:221:ASN:O	1:A:224:LYS:HB2	2.14	0.47
1:A:253:THR:OG1	1:B:75:PRO:HG3	2.15	0.47
1:A:536:LEU:HG	1:B:510:LEU:HD11	1.97	0.47
1:B:324:ILE:HD13	1:B:389:ARG:O	2.15	0.47
1:A:381:SER:OG	4:A:818:HOH:O	2.20	0.47
1:B:456:ALA:O	1:B:460:ILE:HG13	2.15	0.47
1:A:104:LEU:HB3	1:A:112:TYR:OH	2.14	0.47
1:B:443:THR:C	1:B:445:GLU:N	2.67	0.47
1:A:422:GLN:NE2	1:A:503:GLU:OE1	2.48	0.47
1:B:188:LEU:HD23	1:B:188:LEU:HA	1.76	0.47
1:B:163:LEU:O	1:B:166:ALA:HB3	2.14	0.47
1:A:206:ARG:NH1	1:B:427:PHE:CD1	2.82	0.47
1:A:443:THR:C	1:A:445:GLU:N	2.68	0.47
1:B:448:VAL:O	1:B:452:LYS:HG3	2.15	0.47
1:B:104:LEU:HB3	1:B:112:TYR:OH	2.15	0.47
1:A:324:ILE:HD13	1:A:389:ARG:O	2.15	0.47
1:A:456:ALA:O	1:A:460:ILE:HG13	2.15	0.47
1:B:145:ASP:OD1	1:B:296:ARG:HD2	2.15	0.47
1:B:422:GLN:NE2	1:B:503:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:145:ASP:OD1	1:A:296:ARG:HD2	2.15	0.46
1:A:205:GLU:OE1	1:B:428:SER:N	2.39	0.46
1:B:266:GLY:O	1:B:280:LEU:HD22	2.15	0.46
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.77	0.46
1:A:66:ALA:HB1	1:B:260:ILE:HD11	1.96	0.46
1:A:482:GLN:O	1:A:483:LYS:C	2.54	0.46
1:A:448:VAL:O	1:A:452:LYS:HG3	2.15	0.46
1:A:425:ILE:HD13	1:B:209:GLY:HA2	1.96	0.46
1:B:185:LEU:CB	1:B:305:THR:HG21	2.46	0.46
1:A:170:ILE:HG13	1:A:258:GLY:CA	2.44	0.46
1:B:383:LEU:O	1:B:386:LEU:HB2	2.16	0.46
1:B:33:ILE:HB	1:B:34:PRO:HD3	1.98	0.46
1:B:429:ASP:O	1:B:471:VAL:HG22	2.16	0.46
1:A:425:ILE:HG22	1:A:426:LEU:N	2.30	0.46
1:A:364:ILE:HG12	1:A:370:VAL:HG21	1.98	0.46
1:A:2:ILE:HD11	1:A:308:PHE:CE2	2.50	0.46
1:A:61:ILE:O	1:A:65:ILE:HB	2.16	0.46
1:A:485:ARG:HG3	1:A:508:LEU:HD21	1.97	0.46
1:A:357:LEU:HD11	1:A:383:LEU:CA	2.46	0.46
1:B:420:VAL:HG12	1:B:420:VAL:O	2.16	0.46
1:B:221:ASN:O	1:B:224:LYS:HB2	2.15	0.46
1:B:275:ILE:CG2	1:B:276:THR:N	2.79	0.46
1:A:427:PHE:CD1	1:B:206:ARG:NH1	2.84	0.46
1:B:425:ILE:HG22	1:B:426:LEU:N	2.31	0.46
1:B:170:ILE:HG13	1:B:258:GLY:CA	2.45	0.46
1:B:162:LYS:CD	1:B:162:LYS:H	2.23	0.45
1:A:260:ILE:HD11	1:B:66:ALA:HB1	1.98	0.45
3:A:701:ANP:H2'	1:B:477:LYS:O	2.16	0.45
1:A:464:PRO:O	1:A:465:GLN:HB2	2.16	0.45
1:B:485:ARG:HG3	1:B:508:LEU:HD21	1.98	0.45
1:B:558:THR:O	1:B:559:HIS:C	2.54	0.45
1:B:2:ILE:HD11	1:B:308:PHE:CE2	2.51	0.45
1:B:260:ILE:C	1:B:262:VAL:N	2.68	0.45
1:B:156:MET:C	1:B:164:THR:HG21	2.36	0.45
1:A:510:LEU:HD11	1:B:536:LEU:HG	1.98	0.45
1:A:41:ILE:HA	1:A:45:ILE:HD12	1.99	0.45
1:B:364:ILE:HG12	1:B:370:VAL:HG21	1.97	0.45
1:B:508:LEU:HD13	1:B:516:ILE:HD12	1.99	0.45
1:A:383:LEU:O	1:A:386:LEU:HB2	2.17	0.45
1:B:380:LYS:HE3	1:B:380:LYS:HB2	1.49	0.45
1:A:381:SER:HB2	4:A:818:HOH:O	2.14	0.45
1:A:173:PHE:N	1:A:173:PHE:CD1	2.84	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.83	0.45
1:B:267:ALA:C	1:B:269:LEU:N	2.68	0.45
1:A:271:ILE:HD13	1:B:56:VAL:HG22	1.98	0.45
1:A:429:ASP:O	1:A:471:VAL:HG22	2.17	0.45
1:B:276:THR:C	1:B:278:GLY:H	2.20	0.45
1:B:212:VAL:CG1	1:B:213:VAL:N	2.79	0.45
1:A:33:ILE:HB	1:A:34:PRO:HD3	1.98	0.45
1:A:37:ILE:HG13	1:B:263:ILE:HD11	1.98	0.45
1:B:173:PHE:N	1:B:173:PHE:CD1	2.84	0.45
1:A:422:GLN:NE2	1:B:507:ALA:CB	2.80	0.45
1:A:505:THR:O	1:A:506:SER:C	2.55	0.45
1:A:212:VAL:CG1	1:A:213:VAL:N	2.79	0.45
1:B:384:ILE:HD13	1:B:500:ILE:HG23	1.99	0.45
1:B:267:ALA:O	1:B:269:LEU:N	2.50	0.45
1:B:266:GLY:HA3	1:B:280:LEU:HD11	1.98	0.45
1:A:169:PHE:HD2	1:A:261:ILE:HD13	1.82	0.45
1:B:357:LEU:HD11	1:B:383:LEU:CA	2.46	0.44
1:A:539:ILE:HA	1:A:539:ILE:HD12	1.67	0.44
1:A:24:ILE:O	1:A:26:LYS:N	2.51	0.44
1:B:59:LEU:O	1:B:59:LEU:HG	2.17	0.44
1:B:27:PHE:H	1:B:27:PHE:HD1	1.64	0.44
1:B:169:PHE:HD2	1:B:261:ILE:HD13	1.82	0.44
1:B:505:THR:O	1:B:506:SER:C	2.56	0.44
1:B:332:PRO:HD3	1:B:409:LEU:CD1	2.43	0.44
1:A:558:THR:O	1:A:559:HIS:C	2.54	0.44
1:A:202:PHE:CE1	1:A:206:ARG:NE	2.86	0.44
1:B:294:LEU:O	1:B:298:VAL:HG23	2.16	0.44
1:B:482:GLN:O	1:B:483:LYS:C	2.53	0.44
1:A:384:ILE:HD13	1:A:500:ILE:HG23	1.98	0.44
1:B:292:GLY:O	1:B:296:ARG:HG3	2.17	0.44
1:A:466:GLY:O	1:A:468:ASP:N	2.50	0.44
1:A:555:GLU:OE1	1:A:568:ALA:HB3	2.17	0.44
1:A:67:LEU:CD2	1:B:260:ILE:HG21	2.47	0.44
1:B:106:ALA:HB3	1:B:322:TYR:CE2	2.48	0.44
1:A:571:HIS:O	1:A:575:ILE:HG13	2.18	0.44
1:A:420:VAL:O	1:A:420:VAL:HG12	2.16	0.44
1:A:10:LYS:C	1:A:12:TYR:H	2.21	0.44
1:B:202:PHE:CE1	1:B:206:ARG:NE	2.86	0.44
1:A:473:GLU:C	1:A:475:GLY:N	2.71	0.44
1:B:349:TYR:OH	1:B:382:THR:HG23	2.18	0.44
1:B:571:HIS:O	1:B:575:ILE:HG13	2.18	0.44
1:A:275:ILE:HG21	1:A:279:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:202:PHE:CZ	1:B:206:ARG:HG3	2.53	0.44
1:A:332:PRO:HD3	1:A:409:LEU:CD1	2.44	0.44
1:B:27:PHE:N	1:B:27:PHE:CD1	2.86	0.44
1:A:58:HIS:HA	1:A:61:ILE:HG12	2.00	0.44
1:B:570:GLU:C	1:B:570:GLU:OE1	2.56	0.44
1:A:292:GLY:O	1:A:296:ARG:HG3	2.18	0.44
1:A:294:LEU:O	1:A:298:VAL:HG23	2.16	0.44
1:A:169:PHE:CD2	1:A:261:ILE:HD13	2.53	0.43
1:B:169:PHE:CD2	1:B:261:ILE:HD13	2.53	0.43
1:B:466:GLY:O	1:B:468:ASP:N	2.50	0.43
1:B:276:THR:HB	1:B:279:THR:OG1	2.18	0.43
1:A:349:TYR:OH	1:A:382:THR:HG23	2.18	0.43
1:A:171:PHE:HB2	1:A:172:PRO:HD3	2.00	0.43
1:A:477:LYS:HG2	3:B:700:ANP:N6	2.32	0.43
1:B:51:THR:HG22	1:B:52:THR:N	2.33	0.43
1:A:508:LEU:HD13	1:A:516:ILE:HD12	2.00	0.43
1:B:271:ILE:C	1:B:273:GLY:H	2.22	0.43
1:A:190:ARG:HH11	1:A:190:ARG:HG3	1.83	0.43
1:B:244:ASN:OD1	1:B:302:THR:HG23	2.19	0.43
1:B:100:LEU:O	1:B:103:HIS:HB3	2.18	0.43
1:B:509:ASP:OD2	1:B:511:GLU:HB3	2.18	0.43
1:A:27:PHE:H	1:A:27:PHE:HD1	1.64	0.43
1:A:200:GLN:HG2	1:B:125:ILE:HD13	2.00	0.43
1:B:153:LEU:HD23	1:B:153:LEU:HA	1.83	0.43
1:A:509:ASP:OD2	1:A:511:GLU:HB3	2.18	0.43
1:A:202:PHE:CZ	1:A:206:ARG:HG3	2.53	0.43
1:B:24:ILE:O	1:B:26:LYS:N	2.51	0.43
1:A:570:GLU:OE1	1:A:570:GLU:C	2.56	0.43
1:A:267:ALA:HA	1:A:280:LEU:CD2	2.49	0.43
1:B:10:LYS:C	1:B:12:TYR:H	2.21	0.43
1:B:54:GLU:O	1:B:57:HIS:HB3	2.19	0.43
1:B:357:LEU:HD11	1:B:383:LEU:HA	2.01	0.43
1:A:75:PRO:HG3	1:B:253:THR:OG1	2.19	0.43
1:B:34:PRO:HA	1:B:37:ILE:HD12	2.01	0.43
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.86	0.43
1:B:171:PHE:HB2	1:B:172:PRO:HD3	1.99	0.43
1:A:100:LEU:O	1:A:103:HIS:HB3	2.18	0.43
1:B:555:GLU:OE1	1:B:568:ALA:HB3	2.19	0.43
1:A:377:GLY:N	3:A:701:ANP:O1B	2.52	0.43
1:B:190:ARG:HG3	1:B:190:ARG:HH11	1.83	0.43
1:A:2:ILE:O	1:A:6:LEU:HG	2.19	0.42
1:A:453:MET:HB3	1:A:492:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:71:VAL:CG1	1:B:71:VAL:O	2.67	0.42
1:A:29:ILE:N	1:A:30:PRO:HD2	2.34	0.42
1:A:86:GLN:O	1:A:87:TRP:C	2.57	0.42
1:A:244:ASN:OD1	1:A:302:THR:HG23	2.19	0.42
1:B:156:MET:HB3	1:B:156:MET:HE2	1.80	0.42
1:A:549:GLU:O	1:A:550:ASN:C	2.58	0.42
1:A:357:LEU:HD11	1:A:383:LEU:HA	2.01	0.42
1:A:159:LEU:HD23	1:A:283:PHE:CD1	2.53	0.42
1:B:453:MET:HB3	1:B:492:PHE:CD2	2.54	0.42
1:B:269:LEU:HB3	1:B:274:SER:OG	2.19	0.42
1:A:185:LEU:CB	1:A:305:THR:HG21	2.47	0.42
3:A:701:ANP:N3B	1:B:479:SER:OG	2.53	0.42
1:A:104:LEU:C	1:A:106:ALA:H	2.23	0.42
1:B:104:LEU:C	1:B:106:ALA:H	2.23	0.42
1:A:502:ASP:HA	1:A:532:VAL:HB	2.02	0.42
1:A:34:PRO:HA	1:A:37:ILE:HD12	2.02	0.42
1:B:384:ILE:CD1	1:B:500:ILE:HG23	2.50	0.42
1:A:507:ALA:CB	1:B:422:GLN:NE2	2.83	0.42
1:B:86:GLN:O	1:B:87:TRP:C	2.58	0.42
1:A:384:ILE:CD1	1:A:532:VAL:HG23	2.49	0.42
1:B:289:LEU:HD23	1:B:289:LEU:HA	1.83	0.42
1:B:234:LEU:O	1:B:235:THR:C	2.58	0.42
1:B:163:LEU:HG	1:B:283:PHE:CE2	2.55	0.42
1:B:329:GLY:O	1:B:330:ALA:C	2.58	0.42
1:A:329:GLY:O	1:A:330:ALA:C	2.58	0.42
1:B:262:VAL:HG12	1:B:263:ILE:N	2.34	0.42
1:A:422:GLN:HE22	1:B:507:ALA:HB1	1.85	0.42
1:B:365:GLU:N	1:B:368:GLU:OE1	2.47	0.42
1:A:464:PRO:HG3	1:B:353:GLU:CG	2.48	0.42
1:A:284:VAL:HG11	1:B:37:ILE:HG23	2.01	0.42
1:A:422:GLN:NE2	1:B:507:ALA:HB2	2.35	0.42
1:A:290:LEU:HA	1:A:290:LEU:HD23	1.81	0.42
1:B:206:ARG:O	1:B:209:GLY:N	2.52	0.42
1:A:409:LEU:O	1:A:410:THR:C	2.58	0.42
1:A:163:LEU:O	1:A:166:ALA:HB3	2.20	0.42
1:B:356:ILE:O	1:B:551:GLY:HA3	2.20	0.42
1:A:199:VAL:CG2	1:A:200:GLN:N	2.83	0.42
1:B:199:VAL:CG2	1:B:200:GLN:N	2.83	0.42
1:B:110:ARG:O	1:B:111:PHE:C	2.57	0.42
1:B:238:LEU:O	1:B:239:LYS:C	2.59	0.42
1:B:194:GLN:O	1:B:197:ALA:HB3	2.20	0.42
1:B:108:SER:N	4:B:816:HOH:O	2.17	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:701:ANP:C5	1:B:477:LYS:HA	2.50	0.41
1:A:71:VAL:O	1:A:71:VAL:CG1	2.67	0.41
1:A:121:ILE:HD13	1:B:204:HIS:CD2	2.55	0.41
1:B:409:LEU:O	1:B:410:THR:C	2.58	0.41
1:A:480:GLY:HA3	3:B:700:ANP:O2G	2.20	0.41
1:A:480:GLY:CA	3:B:700:ANP:O2G	2.69	0.41
1:A:104:LEU:C	1:A:106:ALA:N	2.73	0.41
1:B:167:ALA:O	1:B:169:PHE:N	2.53	0.41
1:A:10:LYS:HB3	1:A:11:PRO:CD	2.50	0.41
1:A:206:ARG:O	1:A:209:GLY:N	2.52	0.41
1:B:260:ILE:O	1:B:262:VAL:N	2.54	0.41
1:B:29:ILE:N	1:B:30:PRO:HD2	2.35	0.41
1:A:437:LEU:HD12	1:A:490:ARG:NH2	2.35	0.41
1:B:437:LEU:HD12	1:B:490:ARG:NH2	2.35	0.41
1:A:106:ALA:HB3	1:A:322:TYR:CE2	2.48	0.41
1:B:502:ASP:HA	1:B:532:VAL:HB	2.02	0.41
1:A:304:LEU:O	1:A:305:THR:C	2.59	0.41
1:B:479:SER:O	1:B:483:LYS:HG3	2.20	0.41
1:A:479:SER:O	1:A:483:LYS:HG3	2.20	0.41
1:B:259:PRO:HD3	1:B:291:PHE:CD2	2.56	0.41
1:A:439:ARG:NH2	1:A:446:GLU:CD	2.74	0.41
1:B:2:ILE:O	1:B:6:LEU:HG	2.20	0.41
1:A:259:PRO:HD3	1:A:291:PHE:CD2	2.56	0.41
1:B:104:LEU:C	1:B:106:ALA:N	2.73	0.41
1:B:384:ILE:CD1	1:B:532:VAL:HG23	2.50	0.41
1:A:371:ALA:HB1	1:A:539:ILE:CG1	2.51	0.41
1:A:266:GLY:HA3	1:A:280:LEU:HD11	2.01	0.41
1:A:380:LYS:HE3	1:A:380:LYS:HB2	1.50	0.41
1:B:189:THR:HG21	1:B:306:GLN:HA	2.02	0.41
1:A:242:ARG:HG2	1:B:83:TYR:CE1	2.56	0.41
1:A:189:THR:HG21	1:A:306:GLN:HA	2.02	0.41
1:A:472:GLY:O	1:A:473:GLU:C	2.58	0.41
1:A:156:MET:HB3	1:A:283:PHE:HE1	1.85	0.41
1:A:384:ILE:CD1	1:A:500:ILE:HG23	2.50	0.41
1:B:371:ALA:HB1	1:B:539:ILE:CG1	2.51	0.41
1:A:27:PHE:N	1:A:27:PHE:CD1	2.86	0.41
1:A:238:LEU:O	1:A:239:LYS:C	2.59	0.41
1:A:10:LYS:O	1:A:12:TYR:N	2.54	0.41
1:A:260:ILE:O	1:A:263:ILE:N	2.54	0.41
1:A:291:PHE:N	1:A:291:PHE:CD1	2.89	0.41
1:B:25:ILE:CG2	1:B:25:ILE:O	2.67	0.41
1:A:356:ILE:O	1:A:551:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:356:ILE:HD12	3:A:701:ANP:H1'	2.03	0.40
1:B:439:ARG:NH2	1:B:446:GLU:CD	2.74	0.40
1:A:234:LEU:O	1:A:235:THR:C	2.59	0.40
1:B:160:ASP:OD1	1:B:275:ILE:HD11	2.20	0.40
1:B:304:LEU:O	1:B:305:THR:C	2.60	0.40
1:B:443:THR:CB	1:B:446:GLU:HG3	2.50	0.40
1:A:59:LEU:HD21	1:B:267:ALA:HB3	2.04	0.40
1:B:331:GLN:O	1:B:333:ILE:N	2.54	0.40
1:B:265:VAL:O	1:B:269:LEU:HG	2.21	0.40
1:A:110:ARG:O	1:A:111:PHE:C	2.58	0.40
1:A:160:ASP:OD1	1:A:163:LEU:N	2.55	0.40
1:B:181:PHE:CE2	1:B:246:TYR:HD2	2.40	0.40
1:A:181:PHE:CE2	1:A:246:TYR:HD2	2.39	0.40
1:A:200:GLN:HB3	1:A:200:GLN:HE21	1.63	0.40
1:B:570:GLU:O	1:B:571:HIS:C	2.60	0.40
1:A:167:ALA:C	1:A:169:PHE:N	2.74	0.40
1:A:27:PHE:C	1:A:30:PRO:HD2	2.41	0.40
1:B:27:PHE:C	1:B:30:PRO:HD2	2.41	0.40
1:A:194:GLN:O	1:A:197:ALA:HB3	2.22	0.40
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.81	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	576/578 (100%)	463 (80%)	95 (16%)	18 (3%)	7	52
1	B	576/578 (100%)	458 (80%)	102 (18%)	16 (3%)	8	54
All	All	1152/1156 (100%)	921 (80%)	197 (17%)	34 (3%)	7	53

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	338	GLY
1	A	506	SER
1	B	25	ILE
1	B	182	PHE
1	B	338	GLY
1	B	506	SER
1	A	41	ILE
1	A	160	ASP
1	A	168	LEU
1	A	182	PHE
1	A	466	GLY
1	B	466	GLY
1	A	467	TYR
1	A	537	SER
1	B	168	LEU
1	B	268	TYR
1	B	467	TYR
1	B	537	SER
1	A	49	ALA
1	A	88	THR
1	A	250	ALA
1	A	410	THR
1	B	88	THR
1	B	250	ALA
1	B	410	THR
1	A	332	PRO
1	B	332	PRO
1	A	11	PRO
1	B	11	PRO
1	A	10	LYS
1	A	171	PHE
1	B	10	LYS
1	B	171	PHE

### 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	499/499 (100%)	473 (95%)	26 (5%)	32	77
1	B	499/499 (100%)	471 (94%)	28 (6%)	30	75
All	All	998/998 (100%)	944 (95%)	54 (5%)	31	77

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ILE
1	A	82	GLN
1	A	162	LYS
1	A	199	VAL
1	A	200	GLN
1	A	241	THR
1	A	289	LEU
1	A	290	LEU
1	A	295	ARG
1	A	321	ASP
1	A	365	GLU
1	A	373	VAL
1	A	384	ILE
1	A	392	ASP
1	A	393	VAL
1	A	424	ASN
1	A	429	ASP
1	A	443	THR
1	A	474	ARG
1	A	479	SER
1	A	487	SER
1	A	491	ILE
1	A	536	LEU
1	A	539	ILE
1	A	556	THR
1	A	570	GLU
1	B	65	ILE
1	B	82	GLN
1	B	159	LEU
1	B	162	LYS
1	B	199	VAL
1	B	241	THR
1	B	289	LEU
1	B	290	LEU
1	B	295	ARG

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Mol	Chain	Res	Type
1	B	321	ASP
1	B	365	GLU
1	B	373	VAL
1	B	384	ILE
1	B	392	ASP
1	B	393	VAL
1	B	424	ASN
1	B	429	ASP
1	B	443	THR
1	B	474	ARG
1	B	479	SER
1	B	487	SER
1	B	491	ILE
1	B	496	PRO
1	B	536	LEU
1	B	539	ILE
1	B	556	THR
1	B	570	GLU
1	B	578	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	105	GLN
1	A	126	ASN
1	A	200	GLN
1	A	204	HIS
1	A	306	GLN
1	A	397	GLN
1	A	455	ASN
1	A	465	GLN
1	B	47	ASN
1	B	105	GLN
1	B	126	ASN
1	B	200	GLN
1	B	306	GLN
1	B	397	GLN
1	B	424	ASN
1	B	455	ASN
1	B	465	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 6 ligands modelled in this entry, 4 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	$\# Z  > 2$
3	ANP	A	701	2	33,33,33	5.67	25 (75%)	51,52,52	3.92	22 (43%)
3	ANP	B	700	2	33,33,33	5.73	22 (66%)	51,52,52	3.95	23 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	701	2	-	0/18/38/38	0/1/3/3
3	ANP	B	700	2	-	0/18/38/38	0/1/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ANP	PG-O1G	16.41	1.66	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	ANP	PG-O1G	15.22	1.65	1.46
3	B	700	ANP	PB-N3B	14.74	1.77	1.64
3	A	701	ANP	PB-O3A	12.10	1.76	1.59
3	B	700	ANP	PB-O3A	12.06	1.76	1.59
3	A	701	ANP	PG-N3B	11.99	1.74	1.64
3	B	700	ANP	PB-O1B	11.44	1.60	1.46
3	A	701	ANP	PB-N3B	10.53	1.73	1.64
3	A	701	ANP	PB-O1B	10.50	1.59	1.46
3	B	700	ANP	PG-N3B	9.34	1.72	1.64
3	B	700	ANP	PG-O3G	7.44	1.77	1.55
3	A	701	ANP	PG-O3G	7.23	1.76	1.55
3	A	701	ANP	PG-O2G	6.39	1.74	1.55
3	B	700	ANP	PG-O2G	6.26	1.73	1.55
3	B	700	ANP	C2'-C1'	5.16	1.60	1.53
3	A	701	ANP	C2'-C1'	4.62	1.60	1.53
3	B	700	ANP	C2-N1	4.50	1.42	1.33
3	A	701	ANP	PA-O2A	4.43	1.74	1.55
3	A	701	ANP	C2-N1	3.91	1.41	1.33
3	B	700	ANP	O4'-C4'	-3.82	1.36	1.45
3	B	700	ANP	C3'-C4'	3.79	1.63	1.53
3	B	700	ANP	C8-N9	3.78	1.42	1.36
3	A	701	ANP	C3'-C4'	3.68	1.63	1.53
3	B	700	ANP	PA-O2A	3.59	1.71	1.55
3	A	701	ANP	C4-N9	-3.59	1.32	1.37
3	A	701	ANP	C8-N9	3.54	1.41	1.36
3	A	701	ANP	O4'-C4'	-3.34	1.37	1.45
3	A	701	ANP	PA-O3A	-3.11	1.54	1.59
3	A	701	ANP	C2-N3	2.97	1.38	1.32
3	B	700	ANP	C4-N9	-2.87	1.33	1.37
3	B	700	ANP	C8-N7	-2.75	1.29	1.34
3	A	701	ANP	C6-N6	2.75	1.43	1.35
3	A	701	ANP	O5'-C5'	2.72	1.56	1.44
3	A	701	ANP	C2'-C3'	2.70	1.60	1.53
3	A	701	ANP	C8-N7	-2.64	1.29	1.34
3	B	700	ANP	O5'-C5'	2.43	1.54	1.44
3	B	700	ANP	PA-O3A	-2.33	1.55	1.59
3	B	700	ANP	C1'-N9	-2.31	1.41	1.48
3	B	700	ANP	C2'-C3'	2.29	1.59	1.53
3	A	701	ANP	C1'-N9	-2.25	1.41	1.48
3	A	701	ANP	PB-O2B	2.20	1.61	1.55
3	B	700	ANP	C6-N6	2.18	1.42	1.35
3	A	701	ANP	C5-C4	2.15	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	ANP	C2-N3	2.10	1.36	1.32
3	A	701	ANP	C6-N1	2.08	1.46	1.37
3	A	701	ANP	O2'-C2'	2.07	1.48	1.43
3	B	700	ANP	PB-O2B	2.04	1.61	1.55

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ANP	C4'-O4'-C1'	-16.26	92.08	109.75
3	B	700	ANP	C4'-O4'-C1'	-15.86	92.53	109.75
3	A	701	ANP	PB-N3B-PG	-10.61	112.22	130.07
3	B	700	ANP	PB-N3B-PG	-10.39	112.59	130.07
3	B	700	ANP	N3-C2-N1	-10.39	120.03	128.71
3	A	701	ANP	N3-C2-N1	-9.29	120.95	128.71
3	B	700	ANP	PA-O3A-PB	-8.96	101.18	131.81
3	A	701	ANP	PA-O3A-PB	-8.70	102.08	131.81
3	B	700	ANP	O3A-PB-N3B	-6.97	87.24	106.59
3	A	701	ANP	O3A-PB-N3B	-6.86	87.57	106.59
3	B	700	ANP	O3'-C3'-C4'	4.55	124.47	111.08
3	A	701	ANP	O4'-C4'-C5'	4.27	124.60	109.36
3	A	701	ANP	O3'-C3'-C4'	4.14	123.27	111.08
3	B	700	ANP	O4'-C4'-C5'	3.98	123.56	109.36
3	B	700	ANP	N3-C4-N9	3.67	132.07	125.43
3	A	701	ANP	O5'-C5'-C4'	-3.65	95.53	108.94
3	B	700	ANP	C2'-C3'-C4'	-3.62	95.44	102.65
3	A	701	ANP	N3-C4-N9	3.58	131.90	125.43
3	A	701	ANP	C2'-C3'-C4'	-3.47	95.74	102.65
3	B	700	ANP	O5'-C5'-C4'	-3.40	96.46	108.94
3	B	700	ANP	N6-C6-N1	3.30	125.85	119.36
3	A	701	ANP	O4'-C1'-C2'	-3.20	101.87	106.77
3	A	701	ANP	N6-C6-N1	3.17	125.59	119.36
3	B	700	ANP	O5'-PA-O1A	3.15	121.71	109.37
3	B	700	ANP	O4'-C1'-C2'	-3.10	102.02	106.77
3	A	701	ANP	O2G-PG-N3B	-3.08	98.25	106.61
3	B	700	ANP	O2G-PG-N3B	-3.07	98.28	106.61
3	A	701	ANP	O5'-PA-O1A	2.99	121.08	109.37
3	B	700	ANP	O3G-PG-N3B	2.86	114.38	106.61
3	A	701	ANP	O3G-PG-N3B	2.70	113.94	106.61
3	A	701	ANP	O3G-PG-O2G	2.69	115.36	107.66
3	A	701	ANP	O3G-PG-O1G	-2.43	107.36	113.60
3	A	701	ANP	O3'-C3'-C2'	2.42	119.72	111.83
3	A	701	ANP	O1B-PB-N3B	2.34	115.37	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	ANP	O2'-C2'-C1'	2.31	118.22	111.23
3	B	700	ANP	O3'-C3'-C2'	2.28	119.25	111.83
3	B	700	ANP	C2'-C1'-N9	2.21	118.93	113.27
3	B	700	ANP	C5-C6-N6	-2.11	115.94	120.72
3	B	700	ANP	O3G-PG-O2G	2.11	113.71	107.66
3	B	700	ANP	O2B-PB-O3A	2.10	115.12	105.14
3	A	701	ANP	C5-C6-N6	-2.09	115.99	120.72
3	B	700	ANP	C2-N3-C4	2.05	119.86	114.01
3	B	700	ANP	O3G-PG-O1G	-2.02	108.41	113.60
3	A	701	ANP	O2'-C2'-C1'	2.01	117.32	111.23
3	A	701	ANP	C3'-C2'-C1'	-2.01	97.77	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	578/578 (100%)	-0.22	1 (0%) 93 77	55, 120, 187, 200	0
1	B	578/578 (100%)	-0.23	3 (0%) 88 61	52, 117, 194, 200	0
All	All	1156/1156 (100%)	-0.22	4 (0%) 91 73	52, 119, 189, 200	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	TYR	2.4
1	B	48	HIS	2.3
1	B	47	ASN	2.2
1	B	578	LEU	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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	B	910	1/1	0.20	0.68	132,132,132,132	0
2	NA	A	900	1/1	0.19	-0.11	125,125,125,125	0
3	ANP	B	700	31/31	0.20	-0.34	74,74,74,74	0
2	NA	B	901	1/1	0.23	-0.44	64,64,64,64	0
3	ANP	A	701	31/31	0.19	-0.55	80,80,80,80	0
2	NA	A	911	1/1	0.15	-1.19	63,63,63,63	0

## 6.5 Other polymers

There are no such residues in this entry.