Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:23 AM GMT

PDB ID	:	2CVT
Title	:	Structures of Yeast Ribonucleotide Reductase I
Authors	:	Xu, H.; Faber, C.; Uchiki, T.; Fairman, J.W.; Racca, J.; Dealwis, C.
Deposited on	:	2005-06-14
Resolution	:	3.20 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:

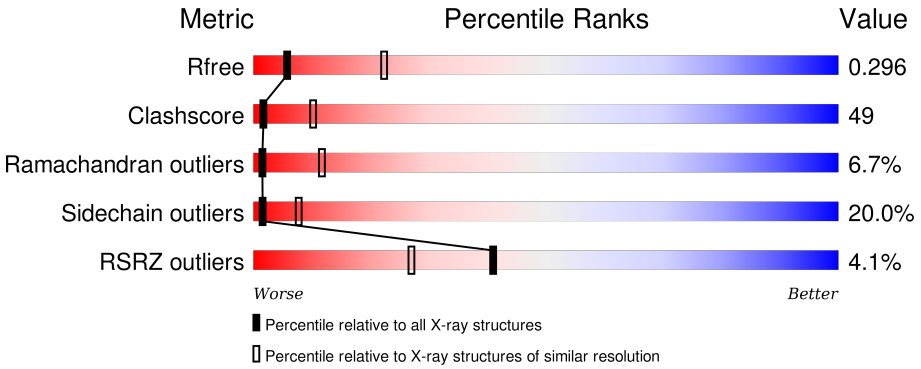
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	888	3%, 21%, 39%, 11%, 28%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5126 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.

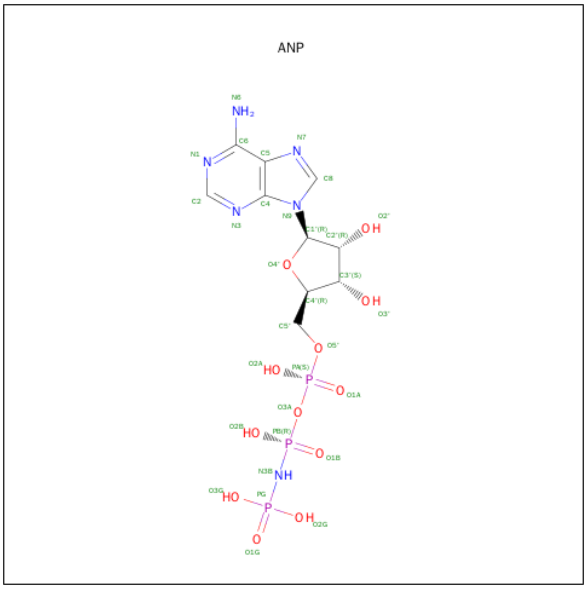
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	0	0	0
			5094	3246	872	947	29			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



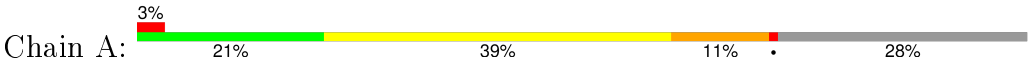
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

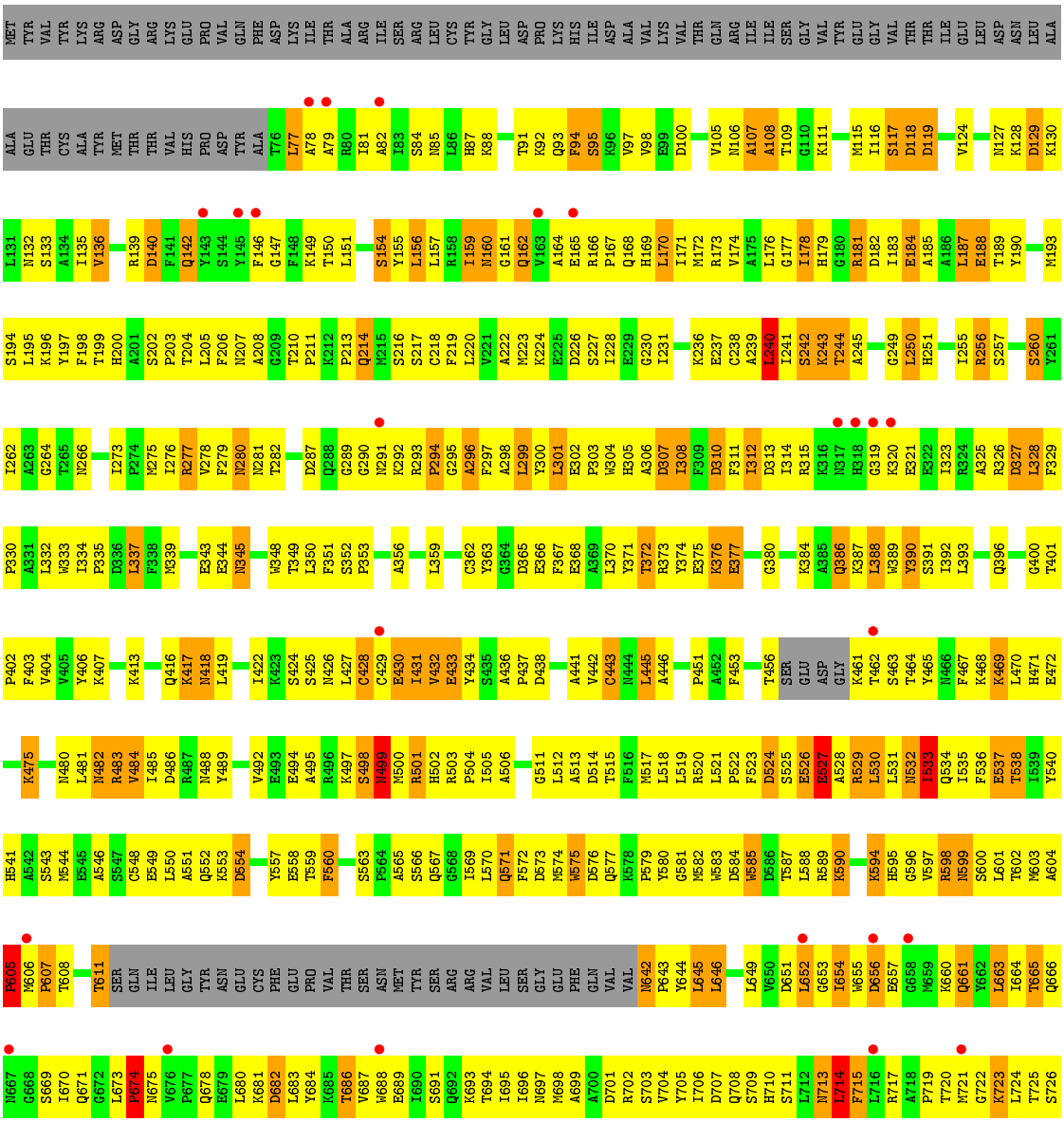
3 Residue-property plots (i)

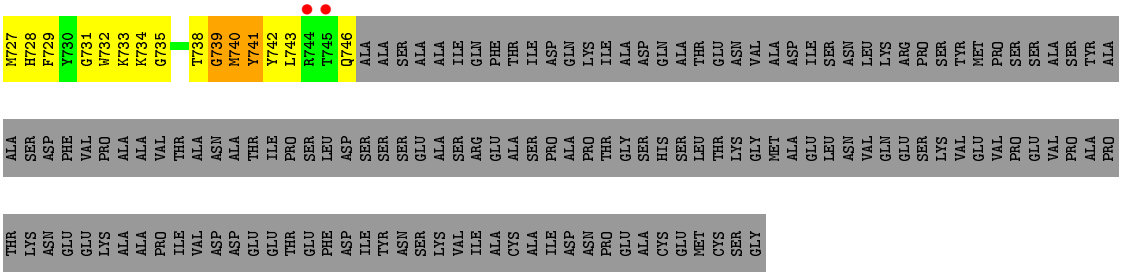
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Ribonucleoside-diphosphate reductase large chain 1

Chain A:






M727 H728 F729 Y730 G731 W732 K733 K734 G735 T738 G739 M740 Y741 Y742 L743 R744 T745 Q746 ALA ALA SER ALA ALA ILE GLN PHE THR ILE ASP GLN LYS ILE ALA ASP GLN ALA THR GLU ASN VAL ALA ASP ILE SER ASN LEU LYS ARG PRO SER TYR MET PRO SER SER ALA SER TYR ALA
ALA SER ASP PHE VAL PRO ALA ALA VAL THR ALA ASN ALA THR ILE PRO SER LEU ASP SER SER SER GLU ALA SER ARG GLU ALA SER PRO ALA PRO THR GLY SER HIS SER LEU THR LYS GLY MET ALA GLU LEU ASN VAL GLN GLU SER LYS VAL GLU VAL PRO GLU VAL PRO ALA PRO
THR LYS ASN GLU GLU LYS ALA ALA PRO ILE VAL ASP ASP GLU GLU THR GLU PHE ASP ILE TYR ASN SER LYS VAL ILE ALA CYS ALA ILE ASP ASN PRO GLU ALA CYS GLU MET CYS SER GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	110.25Å 117.07Å 63.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 40.13 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.9 (50.00-3.20) 92.0 (40.13-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	6.06 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.226 , 0.298 0.226 , 0.296	Depositor DCC
R_{free} test set	655 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	76.8	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 12975 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5126	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: 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	0.86	1/5210 (0.0%)	1.03	21/7050 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	741	TYR	CE1-CZ	-5.41	1.31	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	576	ASP	CB-CG-OD2	7.72	125.25	118.30
1	A	365	ASP	CB-CG-OD2	7.49	125.04	118.30
1	A	714	LEU	CA-CB-CG	7.03	131.46	115.30
1	A	327	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	118	ASP	CB-CG-OD2	6.86	124.48	118.30
1	A	307	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	129	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	483	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	A	119	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	524	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	310	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	651	ASP	CB-CG-OD2	5.78	123.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	656	ASP	N-CA-C	5.67	126.30	111.00
1	A	554	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	682	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	428	CYS	N-CA-C	-5.35	96.56	111.00
1	A	140	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	205	LEU	CB-CG-CD1	-5.28	102.02	111.00
1	A	445	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	328	LEU	CB-CG-CD1	-5.24	102.10	111.00
1	A	77	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	THR	Peptide
1	A	351	PHE	Peptide
1	A	605	PRO	Peptide

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	5094	0	5055	502	0
2	A	1	0	0	0	0
3	A	31	0	13	5	0
All	All	5126	0	5068	504	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 49.

All (504) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASN:HB2	1:A:328:LEU:HD11	1.20	1.20
1:A:699:ALA:HA	1:A:702:ARG:NH1	1.67	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:CG2	1:A:325:ALA:HB2	1.82	1.08
1:A:323:ILE:HG22	1:A:325:ALA:HB2	1.33	1.06
1:A:571:GLN:HE21	1:A:571:GLN:HA	1.13	1.06
1:A:608:THR:HB	1:A:611:THR:HG21	1.36	1.06
1:A:159:ILE:CG2	1:A:160:ASN:H	1.69	1.04
1:A:159:ILE:HG23	1:A:160:ASN:H	0.87	1.04
1:A:550:LEU:HB2	1:A:598:ARG:HG3	1.42	1.02
1:A:159:ILE:HG23	1:A:160:ASN:N	1.69	1.02
1:A:218:CYS:HB2	1:A:443:CYS:SG	2.01	1.01
1:A:571:GLN:NE2	1:A:571:GLN:HA	1.67	1.01
1:A:368:GLU:O	1:A:372:THR:HB	1.61	0.99
1:A:525:SER:HB2	1:A:527:GLU:HG2	1.44	0.99
1:A:181:ARG:HH11	1:A:181:ARG:HG2	1.27	0.97
1:A:505:ILE:HD11	1:A:599:ASN:ND2	1.80	0.96
1:A:537:GLU:HG2	1:A:585:TRP:HH2	1.32	0.95
1:A:238:CYS:HG	1:A:297:PHE:HZ	0.97	0.94
1:A:608:THR:HB	1:A:611:THR:CG2	1.97	0.93
1:A:503:ARG:O	1:A:599:ASN:HB3	1.70	0.92
1:A:661:GLN:O	1:A:664:ILE:HG13	1.70	0.91
3:A:890:ANP:H8	3:A:890:ANP:O1A	1.70	0.91
1:A:181:ARG:HH11	1:A:181:ARG:CG	1.84	0.90
1:A:262:ILE:HG22	1:A:264:GLY:H	1.36	0.90
1:A:717:ARG:O	1:A:719:PRO:HD3	1.71	0.89
1:A:202:SER:HB2	1:A:203:PRO:HD3	1.53	0.88
1:A:699:ALA:HA	1:A:702:ARG:HH12	1.39	0.88
1:A:537:GLU:HG2	1:A:585:TRP:CH2	2.08	0.87
1:A:312:ILE:HG22	1:A:402:PRO:HG3	1.56	0.87
1:A:220:LEU:HD21	1:A:426:ASN:HB3	1.55	0.87
1:A:416:GLN:HE22	1:A:434:TYR:H	1.20	0.85
1:A:541:HIS:CD2	1:A:588:LEU:HD22	2.12	0.84
1:A:214:GLN:HE22	1:A:219:PHE:HZ	1.25	0.82
1:A:533:ILE:HD11	1:A:580:TYR:HB2	1.62	0.82
1:A:608:THR:CB	1:A:611:THR:HG21	2.11	0.81
1:A:323:ILE:HG22	1:A:325:ALA:CB	2.11	0.80
1:A:226:ASP:O	3:A:890:ANP:H5'1	1.82	0.80
1:A:140:ASP:OD2	1:A:168:GLN:HG2	1.80	0.79
1:A:552:GLN:HG2	1:A:595:HIS:CG	2.18	0.79
1:A:238:CYS:SG	1:A:297:PHE:HZ	2.06	0.79
1:A:714:LEU:CD1	1:A:740:MET:HG2	2.13	0.79
1:A:218:CYS:CB	1:A:443:CYS:SG	2.71	0.78
1:A:571:GLN:HE21	1:A:571:GLN:CA	1.92	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:TYR:CG	1:A:580:TYR:O	2.35	0.78
1:A:645:LEU:HD11	1:A:670:ILE:HD13	1.67	0.77
1:A:418:ASN:HD22	1:A:418:ASN:N	1.81	0.77
1:A:224:LYS:HA	1:A:437:PRO:HB3	1.67	0.77
1:A:181:ARG:NH1	1:A:181:ARG:HG2	1.98	0.76
1:A:250:LEU:HD22	1:A:297:PHE:HE1	1.48	0.76
1:A:505:ILE:HD11	1:A:599:ASN:HD22	1.49	0.76
1:A:686:THR:CG2	1:A:688:TRP:HD1	1.97	0.76
1:A:237:GLU:C	1:A:239:ALA:H	1.89	0.76
1:A:77:LEU:HG	1:A:78:ALA:H	1.50	0.76
1:A:575:TRP:CZ2	1:A:703:SER:HB3	2.21	0.76
1:A:255:ILE:HD12	1:A:275:MET:SD	2.26	0.76
1:A:686:THR:HB	1:A:689:GLU:OE1	1.85	0.75
1:A:323:ILE:HG21	1:A:325:ALA:HB2	1.65	0.75
1:A:277:ARG:HG3	1:A:323:ILE:HD13	1.66	0.75
1:A:720:THR:C	1:A:722:GLY:H	1.88	0.75
1:A:396:GLN:O	1:A:400:GLY:N	2.20	0.75
1:A:686:THR:HG23	1:A:688:TRP:HD1	1.52	0.75
1:A:654:ILE:HD11	1:A:675:ASN:HB3	1.68	0.74
1:A:709:SER:OG	1:A:710:HIS:N	2.20	0.73
1:A:106:ASN:OD1	1:A:109:THR:HG23	1.86	0.73
1:A:296:ALA:HB1	1:A:427:LEU:CD2	2.18	0.73
1:A:525:SER:HB2	1:A:527:GLU:CG	2.19	0.73
1:A:537:GLU:OE1	1:A:585:TRP:HZ3	1.71	0.73
1:A:280:ASN:CB	1:A:328:LEU:HD11	2.12	0.73
1:A:709:SER:OG	1:A:738:THR:OG1	1.81	0.72
1:A:475:LYS:HG2	1:A:546:ALA:HB2	1.71	0.72
1:A:256:ARG:HA	1:A:353:PRO:HD2	1.69	0.72
1:A:416:GLN:NE2	1:A:434:TYR:H	1.86	0.72
1:A:522:PRO:HD2	1:A:525:SER:HB3	1.72	0.72
1:A:453:PHE:HD2	1:A:469:LYS:HB3	1.54	0.71
1:A:302:GLU:HG2	1:A:333:TRP:O	1.90	0.71
1:A:552:GLN:HG2	1:A:595:HIS:ND1	2.06	0.71
1:A:572:PHE:CE2	1:A:579:PRO:HD3	2.25	0.71
1:A:740:MET:SD	1:A:742:TYR:N	2.64	0.71
1:A:661:GLN:HA	1:A:661:GLN:NE2	2.05	0.71
1:A:250:LEU:HD22	1:A:297:PHE:CE1	2.25	0.70
1:A:482:ASN:OD1	1:A:503:ARG:NH1	2.24	0.70
1:A:304:TRP:CE2	1:A:359:LEU:HD23	2.25	0.70
1:A:300:TYR:CG	1:A:424:SER:HB2	2.27	0.69
1:A:693:LYS:HE2	1:A:727:MET:CE	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:HD11	1:A:328:LEU:HD22	1.74	0.69
1:A:202:SER:HB2	1:A:203:PRO:CD	2.24	0.68
1:A:590:LYS:O	1:A:590:LYS:HE2	1.94	0.68
1:A:289:GLY:C	1:A:291:ASN:H	1.94	0.68
1:A:604:ALA:HB2	1:A:708:GLN:HG3	1.75	0.68
1:A:293:ARG:HG3	1:A:294:PRO:HD3	1.76	0.67
1:A:241:ILE:O	1:A:243:LYS:N	2.27	0.67
1:A:535:ILE:HG22	1:A:536:PHE:N	2.09	0.67
1:A:709:SER:HG	1:A:738:THR:HG1	0.85	0.67
1:A:207:ASN:ND2	1:A:214:GLN:O	2.25	0.67
1:A:277:ARG:CG	1:A:323:ILE:HD13	2.24	0.67
1:A:214:GLN:HE21	1:A:245:ALA:HA	1.60	0.67
1:A:580:TYR:O	1:A:580:TYR:CD1	2.47	0.67
1:A:418:ASN:N	1:A:418:ASN:ND2	2.42	0.66
1:A:170:LEU:HD22	1:A:173:ARG:NH2	2.10	0.66
1:A:275:MET:O	1:A:278:VAL:HB	1.94	0.66
1:A:699:ALA:HA	1:A:702:ARG:HH11	1.59	0.66
1:A:693:LYS:HE2	1:A:727:MET:HE1	1.78	0.66
1:A:91:THR:HG23	1:A:97:VAL:HG22	1.78	0.66
1:A:210:THR:HB	1:A:211:PRO:CD	2.27	0.65
1:A:429:CYS:O	1:A:738:THR:HG21	1.97	0.65
1:A:504:PRO:C	1:A:505:ILE:HD13	2.17	0.65
3:A:890:ANP:C8	3:A:890:ANP:O1A	2.45	0.64
1:A:428:CYS:HB2	1:A:430:GLU:OE1	1.96	0.64
1:A:179:HIS:HD2	1:A:483:ARG:NH2	1.95	0.64
1:A:280:ASN:HB2	1:A:328:LEU:CD1	2.13	0.64
1:A:301:LEU:HD12	1:A:311:PHE:CG	2.34	0.63
1:A:453:PHE:CD2	1:A:469:LYS:HB3	2.32	0.63
1:A:363:TYR:HA	1:A:367:PHE:HB2	1.79	0.63
1:A:607:PRO:HD2	1:A:608:THR:HG23	1.80	0.62
1:A:167:PRO:O	1:A:171:ILE:HG13	1.99	0.62
1:A:714:LEU:HD13	1:A:740:MET:HG2	1.81	0.62
1:A:577:GLN:NE2	1:A:704:VAL:HG11	2.15	0.62
1:A:418:ASN:ND2	1:A:418:ASN:H	1.98	0.62
1:A:237:GLU:O	1:A:239:ALA:N	2.32	0.62
1:A:471:HIS:HE1	1:A:541:HIS:ND1	1.97	0.62
1:A:200:HIS:HE1	1:A:480:ASN:HB3	1.65	0.61
1:A:77:LEU:HG	1:A:78:ALA:N	2.14	0.61
1:A:505:ILE:N	1:A:505:ILE:HD13	2.14	0.61
1:A:183:ILE:HG22	1:A:187:LEU:HD12	1.83	0.61
1:A:605:PRO:O	1:A:607:PRO:HD3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:MET:SD	1:A:740:MET:C	2.79	0.61
1:A:151:LEU:HD23	1:A:155:TYR:HB2	1.81	0.61
1:A:720:THR:C	1:A:722:GLY:N	2.51	0.61
1:A:531:LEU:HA	1:A:534:GLN:OE1	1.99	0.61
1:A:642:ASN:OD1	1:A:642:ASN:N	2.33	0.60
1:A:446:ALA:N	1:A:481:LEU:HD11	2.17	0.60
1:A:642:ASN:HB2	1:A:645:LEU:HD23	1.82	0.60
1:A:334:ILE:HD12	1:A:404:VAL:HG13	1.83	0.60
1:A:139:ARG:HD3	1:A:194:SER:HB2	1.83	0.60
1:A:560:PHE:O	1:A:563:SER:CB	2.50	0.60
1:A:273:ILE:O	1:A:323:ILE:HD11	2.01	0.60
1:A:534:GLN:HG2	1:A:582:MET:HE3	1.84	0.59
1:A:105:VAL:HG12	1:A:106:ASN:N	2.16	0.59
1:A:502:HIS:ND1	1:A:559:THR:HG21	2.17	0.59
1:A:303:PRO:HA	1:A:308:ILE:HG12	1.84	0.59
1:A:426:ASN:O	1:A:429:CYS:HA	2.03	0.59
1:A:430:GLU:HG2	1:A:431:ILE:N	2.18	0.59
1:A:714:LEU:HD11	1:A:740:MET:HG2	1.84	0.59
1:A:136:VAL:O	1:A:136:VAL:HG22	2.03	0.59
1:A:257:SER:O	1:A:260:SER:HB2	2.03	0.59
1:A:159:ILE:CG2	1:A:160:ASN:N	2.39	0.59
1:A:94:PHE:HA	1:A:169:HIS:CD2	2.38	0.58
1:A:184:GLU:HG3	1:A:185:ALA:H	1.69	0.58
1:A:594:LYS:HD3	1:A:595:HIS:CD2	2.37	0.58
1:A:396:GLN:O	1:A:400:GLY:CA	2.52	0.58
1:A:396:GLN:O	1:A:400:GLY:HA2	2.02	0.58
1:A:649:LEU:HB2	1:A:655:TRP:CZ2	2.39	0.58
1:A:98:VAL:HG21	1:A:124:VAL:HG11	1.84	0.58
1:A:497:LYS:HG3	1:A:501:ARG:HD3	1.86	0.58
1:A:135:ILE:HD11	1:A:172:MET:HG2	1.86	0.58
1:A:325:ALA:HB1	1:A:328:LEU:HD12	1.84	0.58
1:A:179:HIS:HB3	1:A:182:ASP:HB3	1.85	0.58
1:A:231:ILE:HD11	1:A:255:ILE:HD13	1.85	0.58
1:A:363:TYR:HA	1:A:367:PHE:CB	2.33	0.58
1:A:541:HIS:HD2	1:A:588:LEU:HD22	1.68	0.58
1:A:686:THR:HG23	1:A:688:TRP:CD1	2.38	0.58
1:A:654:ILE:O	1:A:655:TRP:CG	2.57	0.58
1:A:255:ILE:CD1	1:A:275:MET:SD	2.91	0.58
1:A:227:SER:HA	3:A:890:ANP:H5'1	1.86	0.57
1:A:325:ALA:O	1:A:327:ASP:N	2.37	0.57
1:A:373:ARG:HA	1:A:376:LYS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:PRO:HD2	1:A:489:TYR:HB2	1.87	0.57
1:A:525:SER:OG	1:A:528:ALA:HB2	2.05	0.57
1:A:106:ASN:OD1	1:A:109:THR:N	2.38	0.57
1:A:107:ALA:O	1:A:108:ALA:HB2	2.05	0.57
1:A:200:HIS:CE1	1:A:480:ASN:HB3	2.40	0.57
1:A:139:ARG:HA	1:A:142:GLN:HG2	1.87	0.57
1:A:297:PHE:HB3	1:A:328:LEU:HD23	1.87	0.56
1:A:574:MET:C	1:A:575:TRP:O	2.40	0.56
1:A:154:SER:O	1:A:206:PHE:HE2	1.89	0.56
1:A:445:LEU:HB3	1:A:506:ALA:HB3	1.87	0.56
1:A:182:ASP:CG	1:A:483:ARG:HH22	2.09	0.56
1:A:362:CYS:HB3	1:A:366:GLU:HG2	1.87	0.56
1:A:289:GLY:C	1:A:291:ASN:N	2.60	0.56
1:A:570:LEU:H	1:A:573:ASP:HB2	1.71	0.55
1:A:367:PHE:C	1:A:367:PHE:CD1	2.80	0.55
1:A:587:THR:O	1:A:590:LYS:HB3	2.06	0.55
1:A:720:THR:O	1:A:722:GLY:N	2.39	0.55
1:A:295:GLY:O	1:A:297:PHE:N	2.40	0.55
1:A:417:LYS:HE3	1:A:574:MET:CE	2.37	0.55
1:A:534:GLN:HG2	1:A:580:TYR:CE1	2.41	0.55
1:A:649:LEU:HD12	1:A:655:TRP:CH2	2.42	0.55
1:A:301:LEU:HD12	1:A:311:PHE:CD1	2.41	0.55
1:A:430:GLU:OE2	1:A:607:PRO:HG2	2.06	0.55
1:A:548:CYS:O	1:A:552:GLN:N	2.34	0.55
1:A:136:VAL:O	1:A:136:VAL:CG2	2.54	0.55
1:A:84:SER:HA	1:A:87:HIS:HB2	1.88	0.55
1:A:106:ASN:HB3	1:A:111:LYS:H	1.72	0.55
1:A:532:ASN:O	1:A:533:ILE:C	2.43	0.54
1:A:513:ALA:O	1:A:517:MET:HE2	2.07	0.54
1:A:571:GLN:NE2	1:A:571:GLN:CA	2.49	0.54
1:A:663:LEU:O	1:A:664:ILE:C	2.45	0.54
1:A:552:GLN:HG2	1:A:595:HIS:CB	2.37	0.54
1:A:187:LEU:O	1:A:190:TYR:HB3	2.06	0.54
1:A:680:LEU:O	1:A:682:ASP:N	2.40	0.54
1:A:94:PHE:CE1	1:A:172:MET:HB3	2.42	0.54
1:A:97:VAL:HG21	1:A:169:HIS:NE2	2.23	0.54
1:A:563:SER:HB3	1:A:566:SER:HB3	1.89	0.54
1:A:575:TRP:CH2	1:A:703:SER:HB3	2.42	0.54
1:A:699:ALA:CA	1:A:702:ARG:HH12	2.17	0.54
1:A:251:HIS:HB3	1:A:424:SER:HB3	1.90	0.54
1:A:663:LEU:HD11	1:A:670:ILE:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HG12	1:A:443:CYS:N	2.23	0.53
1:A:181:ARG:NH1	1:A:181:ARG:CG	2.54	0.53
1:A:396:GLN:HA	1:A:401:THR:H	1.73	0.53
1:A:157:LEU:N	1:A:165:GLU:OE1	2.28	0.53
1:A:214:GLN:NE2	1:A:245:ALA:HA	2.23	0.53
1:A:432:VAL:HG22	1:A:432:VAL:O	2.07	0.53
1:A:502:HIS:C	1:A:504:PRO:HD3	2.28	0.53
1:A:262:ILE:CG2	1:A:264:GLY:H	2.15	0.53
1:A:179:HIS:CD2	1:A:483:ARG:NH2	2.76	0.53
1:A:304:TRP:CE3	1:A:304:TRP:C	2.82	0.53
1:A:645:LEU:CD2	1:A:645:LEU:H	2.22	0.53
1:A:312:ILE:CG2	1:A:402:PRO:HG3	2.35	0.53
1:A:400:GLY:O	1:A:401:THR:CG2	2.56	0.53
1:A:548:CYS:SG	1:A:552:GLN:OE1	2.52	0.53
1:A:384:LYS:O	1:A:387:LYS:N	2.27	0.53
1:A:429:CYS:O	1:A:738:THR:CG2	2.57	0.53
1:A:645:LEU:O	1:A:646:LEU:C	2.47	0.53
1:A:308:ILE:O	1:A:312:ILE:HG12	2.09	0.53
1:A:686:THR:HG22	1:A:689:GLU:H	1.74	0.53
1:A:471:HIS:CE1	1:A:541:HIS:ND1	2.77	0.52
1:A:670:ILE:HD11	1:A:684:TYR:HB2	1.90	0.52
1:A:257:SER:HA	1:A:307:ASP:OD2	2.08	0.52
1:A:227:SER:HA	3:A:890:ANP:C5'	2.39	0.52
1:A:306:ALA:HA	1:A:350:LEU:HB3	1.91	0.52
1:A:348:TRP:CD1	1:A:388:LEU:HD12	2.44	0.52
1:A:524:ASP:O	1:A:525:SER:C	2.47	0.52
1:A:210:THR:HB	1:A:211:PRO:HD2	1.91	0.52
1:A:276:ILE:HG22	1:A:323:ILE:HD12	1.91	0.52
1:A:302:GLU:CG	1:A:333:TRP:O	2.58	0.52
1:A:299:LEU:CD1	1:A:328:LEU:HD22	2.40	0.52
1:A:536:PHE:O	1:A:537:GLU:C	2.47	0.52
1:A:105:VAL:CG1	1:A:106:ASN:N	2.73	0.52
1:A:519:LEU:HB2	1:A:521:LEU:HD12	1.91	0.52
1:A:182:ASP:OD1	1:A:185:ALA:HB2	2.10	0.51
1:A:293:ARG:CG	1:A:294:PRO:HD3	2.41	0.51
1:A:518:LEU:C	1:A:520:ARG:H	2.14	0.51
1:A:182:ASP:OD1	1:A:185:ALA:CB	2.58	0.51
1:A:713:ASN:HA	1:A:742:TYR:O	2.10	0.51
1:A:571:GLN:O	1:A:575:TRP:HD1	1.94	0.51
1:A:582:MET:O	1:A:582:MET:HG2	2.10	0.51
1:A:526:GLU:HA	1:A:529:ARG:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:GLY:O	1:A:654:ILE:HB	2.10	0.51
1:A:220:LEU:HD22	1:A:425:SER:O	2.10	0.51
1:A:179:HIS:HD2	1:A:483:ARG:CZ	2.23	0.51
1:A:579:PRO:C	1:A:581:GLY:H	2.14	0.51
1:A:693:LYS:HE2	1:A:727:MET:HE3	1.93	0.51
1:A:273:ILE:HG13	1:A:310:ASP:HB3	1.92	0.51
1:A:701:ASP:O	1:A:704:VAL:HG22	2.10	0.51
1:A:486:ASP:OD2	1:A:503:ARG:NH2	2.43	0.51
1:A:417:LYS:HE3	1:A:574:MET:HE3	1.93	0.50
1:A:551:ALA:HB2	1:A:597:VAL:C	2.32	0.50
1:A:720:THR:HB	1:A:723:LYS:H	1.77	0.50
1:A:159:ILE:HG22	1:A:162:GLN:O	2.12	0.50
1:A:183:ILE:O	1:A:187:LEU:HD12	2.11	0.50
1:A:484:VAL:O	1:A:488:ASN:HB2	2.11	0.50
1:A:673:LEU:O	1:A:674:PRO:C	2.49	0.50
1:A:216:SER:HB3	1:A:442:VAL:CG1	2.42	0.50
1:A:170:LEU:HD13	1:A:174:VAL:HG23	1.93	0.50
1:A:719:PRO:HB2	1:A:724:LEU:HD21	1.93	0.50
1:A:334:ILE:CD1	1:A:404:VAL:HG13	2.42	0.50
1:A:257:SER:CB	1:A:306:ALA:HB3	2.42	0.50
1:A:106:ASN:O	1:A:108:ALA:N	2.44	0.50
1:A:204:THR:O	1:A:208:ALA:HB2	2.12	0.50
1:A:538:THR:HB	1:A:583:TRP:NE1	2.27	0.50
1:A:93:GLN:O	1:A:94:PHE:C	2.49	0.50
1:A:400:GLY:C	1:A:401:THR:HG23	2.31	0.50
1:A:183:ILE:HG22	1:A:187:LEU:CD1	2.42	0.50
1:A:218:CYS:CB	1:A:443:CYS:HG	2.25	0.49
1:A:337:LEU:HG	1:A:368:GLU:HG2	1.94	0.49
1:A:549:GLU:HA	1:A:552:GLN:HB2	1.93	0.49
1:A:250:LEU:HD21	1:A:299:LEU:CD2	2.42	0.49
1:A:738:THR:O	1:A:739:GLY:O	2.30	0.49
1:A:304:TRP:HB3	1:A:348:TRP:CZ2	2.47	0.49
1:A:557:TYR:CZ	1:A:600:SER:HB3	2.47	0.49
1:A:202:SER:HB3	1:A:206:PHE:CE1	2.48	0.49
1:A:170:LEU:C	1:A:170:LEU:CD1	2.80	0.49
1:A:130:LYS:CB	1:A:130:LYS:NZ	2.76	0.49
1:A:540:TYR:O	1:A:544:MET:HB2	2.13	0.49
1:A:605:PRO:C	1:A:607:PRO:HD3	2.33	0.49
1:A:503:ARG:N	1:A:504:PRO:HD3	2.27	0.49
1:A:262:ILE:HG22	1:A:264:GLY:N	2.17	0.49
1:A:202:SER:CB	1:A:203:PRO:HD3	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ASP:O	1:A:517:MET:N	2.46	0.49
1:A:481:LEU:HB3	1:A:505:ILE:HG23	1.95	0.48
1:A:218:CYS:N	1:A:443:CYS:SG	2.85	0.48
1:A:166:ARG:HD2	1:A:169:HIS:HE1	1.78	0.48
1:A:560:PHE:O	1:A:563:SER:HB2	2.13	0.48
1:A:204:THR:O	1:A:208:ALA:CB	2.61	0.48
1:A:226:ASP:OD2	1:A:256:ARG:HG2	2.14	0.48
1:A:686:THR:CG2	1:A:688:TRP:CD1	2.88	0.48
1:A:518:LEU:C	1:A:520:ARG:N	2.67	0.48
1:A:714:LEU:HD21	1:A:740:MET:HG3	1.95	0.48
1:A:654:ILE:O	1:A:655:TRP:CD1	2.67	0.48
1:A:298:ALA:HB2	1:A:427:LEU:HD13	1.94	0.48
1:A:300:TYR:CB	1:A:424:SER:HB2	2.43	0.48
1:A:406:TYR:HE1	1:A:739:GLY:HA2	1.76	0.48
1:A:470:LEU:O	1:A:471:HIS:C	2.52	0.48
1:A:238:CYS:SG	1:A:297:PHE:CZ	2.94	0.48
1:A:222:ALA:O	1:A:224:LYS:N	2.47	0.48
1:A:691:SER:O	1:A:695:ILE:HG13	2.14	0.48
1:A:582:MET:O	1:A:582:MET:CG	2.62	0.48
1:A:429:CYS:SG	1:A:741:TYR:CE1	3.07	0.48
1:A:530:LEU:O	1:A:533:ILE:HG23	2.13	0.48
1:A:386:GLN:O	1:A:390:TYR:HB2	2.14	0.48
1:A:680:LEU:C	1:A:682:ASP:H	2.18	0.47
1:A:350:LEU:O	1:A:380:GLY:HA3	2.14	0.47
1:A:535:ILE:O	1:A:538:THR:HG23	2.14	0.47
1:A:109:THR:OG1	1:A:111:LYS:HG3	2.14	0.47
1:A:117:SER:O	1:A:118:ASP:C	2.52	0.47
1:A:431:ILE:HG13	1:A:433:GLU:HG3	1.97	0.47
1:A:548:CYS:O	1:A:549:GLU:C	2.52	0.47
1:A:608:THR:CG2	1:A:611:THR:HG21	2.45	0.47
1:A:304:TRP:O	1:A:304:TRP:HE3	1.97	0.47
1:A:713:ASN:O	1:A:715:PHE:CD1	2.67	0.47
1:A:428:CYS:HB3	1:A:607:PRO:HB2	1.97	0.47
1:A:469:LYS:HD3	1:A:469:LYS:HA	1.50	0.47
1:A:166:ARG:HD2	1:A:169:HIS:CE1	2.49	0.47
1:A:497:LYS:CG	1:A:501:ARG:HD3	2.44	0.47
1:A:520:ARG:HG3	1:A:683:LEU:HD21	1.96	0.47
1:A:588:LEU:C	1:A:590:LYS:N	2.68	0.47
1:A:210:THR:CB	1:A:211:PRO:CD	2.91	0.47
1:A:514:ASP:O	1:A:515:THR:C	2.51	0.47
1:A:693:LYS:CE	1:A:727:MET:HE3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:TYR:HE1	1:A:559:THR:HG23	1.80	0.47
1:A:372:THR:HG22	1:A:373:ARG:N	2.29	0.47
1:A:95:SER:OG	1:A:132:ASN:ND2	2.43	0.47
1:A:106:ASN:CG	1:A:109:THR:HG23	2.34	0.47
1:A:560:PHE:O	1:A:563:SER:HB3	2.15	0.47
1:A:344:GLU:HG3	1:A:344:GLU:O	2.15	0.47
1:A:179:HIS:CD2	1:A:483:ARG:CZ	2.99	0.46
1:A:183:ILE:CG2	1:A:187:LEU:HD12	2.45	0.46
1:A:537:GLU:OE1	1:A:585:TRP:CZ3	2.60	0.46
1:A:179:HIS:CE1	1:A:189:THR:OG1	2.68	0.46
1:A:537:GLU:OE2	1:A:582:MET:HB3	2.15	0.46
1:A:344:GLU:O	1:A:345:ASN:C	2.54	0.46
1:A:85:ASN:OD1	1:A:88:LYS:HD2	2.16	0.46
1:A:406:TYR:CE1	1:A:739:GLY:CA	2.98	0.46
1:A:451:PRO:HD3	1:A:511:GLY:HA3	1.98	0.46
1:A:603:MET:O	1:A:708:GLN:HB2	2.16	0.46
1:A:731:GLY:HA2	1:A:734:LYS:HB2	1.98	0.46
1:A:422:ILE:HG21	1:A:432:VAL:HG23	1.97	0.46
1:A:182:ASP:CB	1:A:483:ARG:HH22	2.29	0.45
1:A:403:PHE:CD1	1:A:741:TYR:HE1	2.34	0.45
1:A:663:LEU:HD11	1:A:670:ILE:HG22	1.98	0.45
1:A:250:LEU:HD21	1:A:299:LEU:HD23	1.98	0.45
1:A:222:ALA:HA	1:A:251:HIS:CE1	2.51	0.45
1:A:403:PHE:CD1	1:A:741:TYR:CE1	3.05	0.45
1:A:664:ILE:HD12	1:A:665:THR:N	2.30	0.45
1:A:467:PHE:CD1	1:A:582:MET:SD	3.10	0.45
1:A:719:PRO:CB	1:A:724:LEU:HD21	2.45	0.45
1:A:728:HIS:O	1:A:732:TRP:HB2	2.17	0.45
1:A:498:SER:O	1:A:500:MET:N	2.49	0.45
1:A:695:ILE:O	1:A:696:ILE:C	2.54	0.45
1:A:666:GLN:HE21	1:A:669:SER:HB3	1.82	0.45
1:A:579:PRO:HB2	1:A:581:GLY:H	1.82	0.45
1:A:548:CYS:HG	1:A:552:GLN:CD	2.11	0.45
1:A:605:PRO:HG2	1:A:706:ILE:CD1	2.47	0.45
1:A:323:ILE:HG22	1:A:325:ALA:CA	2.46	0.45
1:A:219:PHE:CE1	1:A:245:ALA:HB1	2.51	0.45
1:A:549:GLU:O	1:A:553:LYS:N	2.37	0.45
1:A:696:ILE:HD11	1:A:714:LEU:HD12	1.99	0.44
1:A:178:ILE:HG22	1:A:483:ARG:HB2	1.98	0.44
1:A:600:SER:C	1:A:601:LEU:HD12	2.37	0.44
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLN:HG3	1:A:601:LEU:HD11	1.98	0.44
1:A:680:LEU:HD22	1:A:684:TYR:CE1	2.52	0.44
1:A:147:GLY:O	1:A:150:THR:HB	2.16	0.44
1:A:241:ILE:C	1:A:243:LYS:H	2.20	0.44
1:A:525:SER:OG	1:A:528:ALA:CB	2.65	0.44
1:A:501:ARG:NH1	1:A:501:ARG:HB3	2.33	0.44
1:A:356:ALA:HB1	1:A:374:TYR:CD1	2.52	0.44
1:A:654:ILE:O	1:A:655:TRP:CB	2.64	0.44
1:A:166:ARG:HB2	1:A:169:HIS:ND1	2.33	0.44
1:A:159:ILE:HB	1:A:164:ALA:HB2	1.98	0.44
1:A:249:GLY:HA2	1:A:298:ALA:O	2.18	0.44
1:A:156:LEU:HG	1:A:165:GLU:O	2.17	0.44
1:A:178:ILE:CG2	1:A:483:ARG:HB2	2.48	0.44
1:A:453:PHE:CZ	1:A:470:LEU:HD12	2.53	0.44
1:A:584:ASP:OD2	1:A:587:THR:HG23	2.18	0.44
1:A:426:ASN:O	1:A:428:CYS:O	2.36	0.43
1:A:522:PRO:HD2	1:A:525:SER:CB	2.46	0.43
1:A:530:LEU:O	1:A:531:LEU:C	2.56	0.43
1:A:400:GLY:O	1:A:401:THR:HG22	2.18	0.43
1:A:569:ILE:C	1:A:570:LEU:HD23	2.38	0.43
1:A:127:ASN:O	1:A:129:ASP:N	2.51	0.43
1:A:663:LEU:O	1:A:666:GLN:O	2.36	0.43
1:A:315:ARG:NH1	1:A:328:LEU:O	2.51	0.43
1:A:189:THR:O	1:A:193:MET:HG3	2.18	0.43
1:A:525:SER:C	1:A:527:GLU:H	2.20	0.43
1:A:214:GLN:HE21	1:A:245:ALA:CA	2.30	0.43
1:A:188:GLU:C	1:A:190:TYR:N	2.69	0.43
1:A:195:LEU:O	1:A:197:TYR:N	2.51	0.43
1:A:605:PRO:HD2	1:A:710:HIS:HB3	2.00	0.43
1:A:400:GLY:C	1:A:401:THR:CG2	2.86	0.43
1:A:250:LEU:CD2	1:A:299:LEU:CD2	2.96	0.43
1:A:406:TYR:CE1	1:A:739:GLY:HA2	2.52	0.43
1:A:695:ILE:C	1:A:697:ASN:N	2.70	0.43
1:A:181:ARG:HA	1:A:181:ARG:HD3	1.82	0.43
1:A:579:PRO:C	1:A:581:GLY:N	2.72	0.43
1:A:551:ALA:HB2	1:A:598:ARG:N	2.33	0.43
1:A:241:ILE:C	1:A:243:LYS:N	2.70	0.43
1:A:279:PHE:C	1:A:281:ASN:H	2.22	0.43
1:A:251:HIS:O	1:A:251:HIS:CD2	2.72	0.43
1:A:696:ILE:O	1:A:699:ALA:HB3	2.18	0.43
1:A:738:THR:C	1:A:739:GLY:O	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:SER:HA	1:A:353:PRO:HD3	1.76	0.43
1:A:304:TRP:C	1:A:304:TRP:HE3	2.21	0.43
1:A:483:ARG:O	1:A:486:ASP:N	2.39	0.43
1:A:663:LEU:HD11	1:A:670:ILE:HG23	2.01	0.43
1:A:305:HIS:O	1:A:308:ILE:HB	2.19	0.43
1:A:392:ILE:O	1:A:393:LEU:C	2.56	0.43
1:A:329:PHE:HA	1:A:330:PRO:HD3	1.85	0.43
1:A:436:ALA:HB1	1:A:437:PRO:HD2	2.01	0.42
1:A:332:LEU:CD1	1:A:392:ILE:HD13	2.49	0.42
1:A:485:ILE:HD11	1:A:505:ILE:CD1	2.49	0.42
1:A:237:GLU:HG2	1:A:492:VAL:HG11	2.02	0.42
1:A:691:SER:O	1:A:694:THR:OG1	2.31	0.42
1:A:185:ALA:O	1:A:189:THR:HG23	2.19	0.42
1:A:304:TRP:CD2	1:A:359:LEU:HD23	2.54	0.42
1:A:81:ILE:HD12	1:A:82:ALA:N	2.35	0.42
1:A:588:LEU:O	1:A:590:LYS:N	2.53	0.42
1:A:296:ALA:HB1	1:A:427:LEU:HD22	1.97	0.42
1:A:130:LYS:C	1:A:133:SER:OG	2.57	0.42
1:A:426:ASN:ND2	1:A:430:GLU:OE1	2.49	0.42
1:A:661:GLN:HA	1:A:661:GLN:HE21	1.80	0.42
1:A:503:ARG:HD3	1:A:598:ARG:O	2.20	0.42
1:A:250:LEU:CD2	1:A:299:LEU:HD23	2.50	0.42
1:A:371:TYR:O	1:A:375:GLU:HG3	2.19	0.42
1:A:230:GLY:O	1:A:231:ILE:C	2.58	0.42
1:A:652:LEU:H	1:A:652:LEU:HG	1.58	0.42
1:A:697:ASN:O	1:A:698:MET:C	2.57	0.42
1:A:572:PHE:CD2	1:A:579:PRO:HD3	2.55	0.42
1:A:713:ASN:O	1:A:715:PHE:HD1	2.03	0.42
1:A:467:PHE:CE1	1:A:582:MET:HE1	2.55	0.42
1:A:588:LEU:HD12	1:A:588:LEU:HA	1.86	0.42
1:A:339:MET:SD	1:A:389:TRP:HZ3	2.43	0.42
1:A:453:PHE:HB2	1:A:465:TYR:CE2	2.55	0.41
1:A:335:PRO:HB3	1:A:407:LYS:HD3	2.02	0.41
1:A:325:ALA:CB	1:A:328:LEU:HD12	2.49	0.41
1:A:94:PHE:CZ	1:A:172:MET:HG3	2.55	0.41
1:A:300:TYR:OH	1:A:429:CYS:SG	2.71	0.41
1:A:453:PHE:HB2	1:A:465:TYR:CZ	2.55	0.41
1:A:740:MET:SD	1:A:741:TYR:N	2.93	0.41
1:A:503:ARG:N	1:A:504:PRO:CD	2.83	0.41
1:A:541:HIS:CD2	1:A:588:LEU:CD2	2.95	0.41
1:A:308:ILE:HD11	1:A:332:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PHE:HA	1:A:441:ALA:O	2.20	0.41
1:A:725:THR:O	1:A:729:PHE:HD1	2.03	0.41
1:A:693:LYS:O	1:A:697:ASN:HB2	2.20	0.41
1:A:481:LEU:HD23	1:A:481:LEU:HA	1.76	0.41
1:A:485:ILE:HG23	1:A:499:ASN:ND2	2.36	0.41
1:A:91:THR:CG2	1:A:97:VAL:HG22	2.50	0.41
1:A:575:TRP:CD1	1:A:704:VAL:HA	2.55	0.41
1:A:94:PHE:HD1	1:A:169:HIS:CD2	2.38	0.41
1:A:92:LYS:HA	1:A:166:ARG:NH2	2.36	0.41
1:A:565:ALA:C	1:A:567:GLN:N	2.72	0.41
1:A:714:LEU:HD11	1:A:740:MET:CG	2.48	0.41
1:A:671:GLN:HG2	1:A:689:GLU:OE2	2.20	0.41
1:A:541:HIS:NE2	1:A:588:LEU:HD22	2.35	0.41
1:A:202:SER:CB	1:A:203:PRO:CD	2.88	0.41
1:A:107:ALA:O	1:A:108:ALA:CB	2.68	0.41
1:A:170:LEU:HD22	1:A:173:ARG:HH21	1.85	0.41
1:A:363:TYR:CA	1:A:367:PHE:HB2	2.48	0.41
1:A:130:LYS:O	1:A:133:SER:OG	2.39	0.41
1:A:85:ASN:HA	1:A:88:LYS:HD2	2.03	0.41
1:A:602:THR:N	1:A:707:ASP:OD2	2.54	0.41
1:A:176:LEU:O	1:A:177:GLY:C	2.59	0.41
1:A:343:GLU:OE2	1:A:733:LYS:HE3	2.21	0.41
1:A:588:LEU:C	1:A:590:LYS:H	2.23	0.41
1:A:536:PHE:CD2	1:A:536:PHE:N	2.89	0.41
1:A:552:GLN:CG	1:A:595:HIS:ND1	2.81	0.41
1:A:296:ALA:HB1	1:A:427:LEU:HD21	1.97	0.41
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.55	0.41
1:A:413:LYS:NZ	1:A:735:GLY:O	2.53	0.41
1:A:198:PHE:CD2	1:A:198:PHE:C	2.94	0.41
1:A:649:LEU:HB2	1:A:655:TRP:CE2	2.56	0.41
1:A:740:MET:SD	1:A:742:TYR:C	2.99	0.40
1:A:467:PHE:HD1	1:A:582:MET:SD	2.44	0.40
1:A:470:LEU:C	1:A:472:GLU:N	2.74	0.40
1:A:541:HIS:CE1	1:A:583:TRP:HB3	2.55	0.40
1:A:678:GLN:HG3	1:A:682:ASP:OD1	2.21	0.40
1:A:308:ILE:HG21	1:A:388:LEU:HD11	2.03	0.40
1:A:183:ILE:CG2	1:A:187:LEU:CD1	2.99	0.40
1:A:429:CYS:HB3	1:A:738:THR:HG23	2.03	0.40
1:A:417:LYS:HE3	1:A:574:MET:HE1	2.02	0.40
1:A:642:ASN:HA	1:A:643:PRO:HD3	1.92	0.40
1:A:312:ILE:HD13	1:A:312:ILE:HG21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLY:O	1:A:401:THR:HG23	2.22	0.40
1:A:213:PRO:CD	1:A:489:TYR:HB2	2.52	0.40
1:A:494:GLU:O	1:A:495:ALA:C	2.58	0.40
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.81	0.40
1:A:375:GLU:O	1:A:376:LYS:C	2.60	0.40
1:A:534:GLN:O	1:A:537:GLU:HB3	2.20	0.40
1:A:305:HIS:ND1	1:A:307:ASP:HB2	2.36	0.40
1:A:293:ARG:N	1:A:294:PRO:HD2	2.36	0.40
1:A:518:LEU:HD21	1:A:644:TYR:OH	2.21	0.40
1:A:127:ASN:O	1:A:128:LYS:C	2.59	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	631/888 (71%)	463 (73%)	126 (20%)	42 (7%)	1 12

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	ALA
1	A	196	LYS
1	A	223	MET
1	A	242	SER
1	A	296	ALA
1	A	314	ILE
1	A	532	ASN
1	A	605	PRO
1	A	607	PRO
1	A	656	ASP
1	A	674	PRO

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Mol	Chain	Res	Type
1	A	721	MET
1	A	94	PHE
1	A	107	ALA
1	A	240	LEU
1	A	321	GLU
1	A	326	ARG
1	A	345	ASN
1	A	376	LYS
1	A	499	ASN
1	A	654	ILE
1	A	665	THR
1	A	681	LYS
1	A	161	GLY
1	A	280	ASN
1	A	290	GLY
1	A	484	VAL
1	A	498	SER
1	A	527	GLU
1	A	575	TRP
1	A	589	ARG
1	A	79	ALA
1	A	119	ASP
1	A	217	SER
1	A	377	GLU
1	A	533	ILE
1	A	606	MET
1	A	646	LEU
1	A	159	ILE
1	A	319	GLY
1	A	294	PRO
1	A	739	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	550/761 (72%)	440 (80%)	110 (20%)	1 8

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	SER
1	A	100	ASP
1	A	115	MET
1	A	116	ILE
1	A	117	SER
1	A	136	VAL
1	A	142	GLN
1	A	146	PHE
1	A	149	LYS
1	A	154	SER
1	A	156	LEU
1	A	160	ASN
1	A	162	GLN
1	A	170	LEU
1	A	178	ILE
1	A	181	ARG
1	A	184	GLU
1	A	187	LEU
1	A	188	GLU
1	A	199	THR
1	A	214	GLN
1	A	228	ILE
1	A	236	LYS
1	A	240	LEU
1	A	242	SER
1	A	243	LYS
1	A	244	THR
1	A	250	LEU
1	A	256	ARG
1	A	260	SER
1	A	266	ASN
1	A	277	ARG
1	A	282	THR
1	A	287	ASP
1	A	292	LYS

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Mol	Chain	Res	Type
1	A	299	LEU
1	A	301	LEU
1	A	308	ILE
1	A	312	ILE
1	A	313	ASP
1	A	320	LYS
1	A	337	LEU
1	A	349	THR
1	A	370	LEU
1	A	372	THR
1	A	377	GLU
1	A	386	GLN
1	A	388	LEU
1	A	390	TYR
1	A	391	SER
1	A	417	LYS
1	A	418	ASN
1	A	419	LEU
1	A	430	GLU
1	A	431	ILE
1	A	432	VAL
1	A	433	GLU
1	A	438	ASP
1	A	443	CYS
1	A	456	THR
1	A	461	LYS
1	A	462	THR
1	A	463	SER
1	A	464	THR
1	A	468	LYS
1	A	469	LYS
1	A	475	LYS
1	A	482	ASN
1	A	499	ASN
1	A	501	ARG
1	A	512	LEU
1	A	523	PHE
1	A	526	GLU
1	A	527	GLU
1	A	529	ARG
1	A	530	LEU
1	A	533	ILE

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Mol	Chain	Res	Type
1	A	537	GLU
1	A	538	THR
1	A	543	SER
1	A	554	ASP
1	A	558	GLU
1	A	560	PHE
1	A	571	GLN
1	A	585	TRP
1	A	590	LYS
1	A	594	LYS
1	A	598	ARG
1	A	599	ASN
1	A	611	THR
1	A	642	ASN
1	A	645	LEU
1	A	652	LEU
1	A	657	GLU
1	A	660	LYS
1	A	661	GLN
1	A	663	LEU
1	A	674	PRO
1	A	686	THR
1	A	687	VAL
1	A	705	TYR
1	A	711	SER
1	A	713	ASN
1	A	714	LEU
1	A	715	PHE
1	A	723	LYS
1	A	726	SER
1	A	740	MET
1	A	743	LEU
1	A	746	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	179	HIS
1	A	251	HIS
1	A	345	ASN
1	A	416	GLN

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Mol	Chain	Res	Type
1	A	418	ASN
1	A	471	HIS
1	A	499	ASN
1	A	532	ASN
1	A	571	GLN
1	A	661	GLN
1	A	666	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	890	2	27,33,33	1.90	5 (18%)	30,52,52	3.05	10 (33%)

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	890	2	-	0/12/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	890	ANP	O4'-C1'	2.05	1.43	1.41
3	A	890	ANP	PB-O3A	2.40	1.62	1.59
3	A	890	ANP	C5-C4	3.28	1.47	1.40
3	A	890	ANP	PG-O1G	4.87	1.51	1.46
3	A	890	ANP	PB-O1B	5.62	1.52	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	890	ANP	O1G-PG-N3B	-10.39	95.96	111.90
3	A	890	ANP	N3-C2-N1	-7.44	123.20	128.89
3	A	890	ANP	O1B-PB-N3B	-4.06	105.68	111.90
3	A	890	ANP	PA-O3A-PB	-3.88	119.66	132.67
3	A	890	ANP	C2'-C1'-N9	-2.53	110.42	114.29
3	A	890	ANP	N6-C6-N1	2.44	124.44	119.20
3	A	890	ANP	C2-N1-C6	2.61	123.43	118.77
3	A	890	ANP	O3G-PG-O2G	3.46	117.85	107.58
3	A	890	ANP	O4'-C1'-N9	3.80	116.06	108.10
3	A	890	ANP	O2B-PB-O1B	4.21	118.79	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	890	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	637/888 (71%)	0.06	26 (4%) 41 27	54, 78, 129, 154	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	656	ASP	5.0
1	A	145	TYR	4.3
1	A	146	PHE	3.9
1	A	320	LYS	3.5
1	A	658	GLY	3.4
1	A	721	MET	3.3
1	A	667	ASN	3.0
1	A	318	HIS	2.9
1	A	82	ALA	2.7
1	A	716	LEU	2.5
1	A	462	THR	2.5
1	A	319	GLY	2.5
1	A	429	CYS	2.4
1	A	652	LEU	2.4
1	A	606	MET	2.3
1	A	79	ALA	2.3
1	A	291	ASN	2.3
1	A	165	GLU	2.1
1	A	143	TYR	2.1
1	A	688	TRP	2.1
1	A	676	VAL	2.1
1	A	317	ASN	2.1
1	A	745	THR	2.0
1	A	78	ALA	2.0
1	A	744	ARG	2.0
1	A	163	VAL	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, 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
3	ANP	A	890	31/31	0.94	0.15	-0.84	83,87,101,103	0
2	MG	A	889	1/1	0.80	0.25	-	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.