



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:59 AM UTC

PDB ID : 2CVT / pdb_00002cvt
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

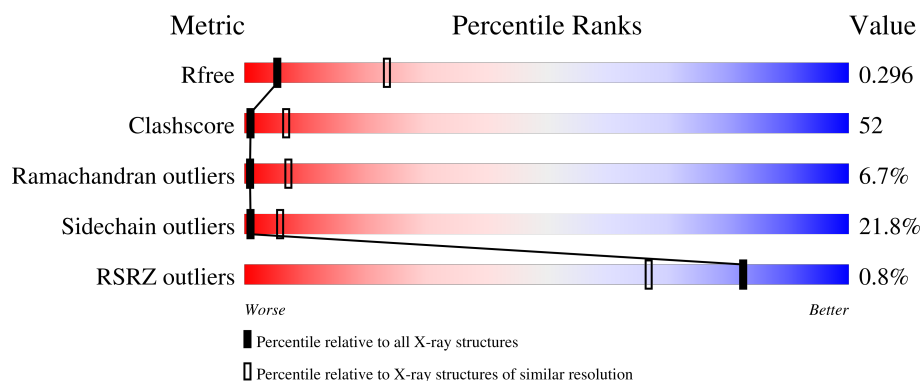
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	888	19%38%13%•28%

2 Entry composition [i](#)

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.

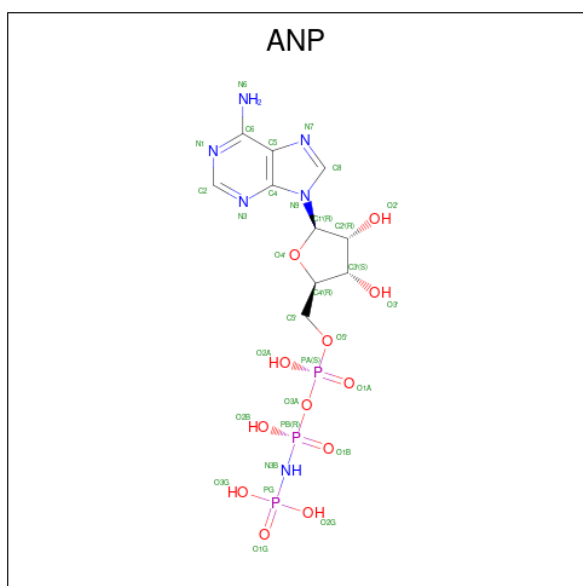
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

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 (CCD ID: 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 (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

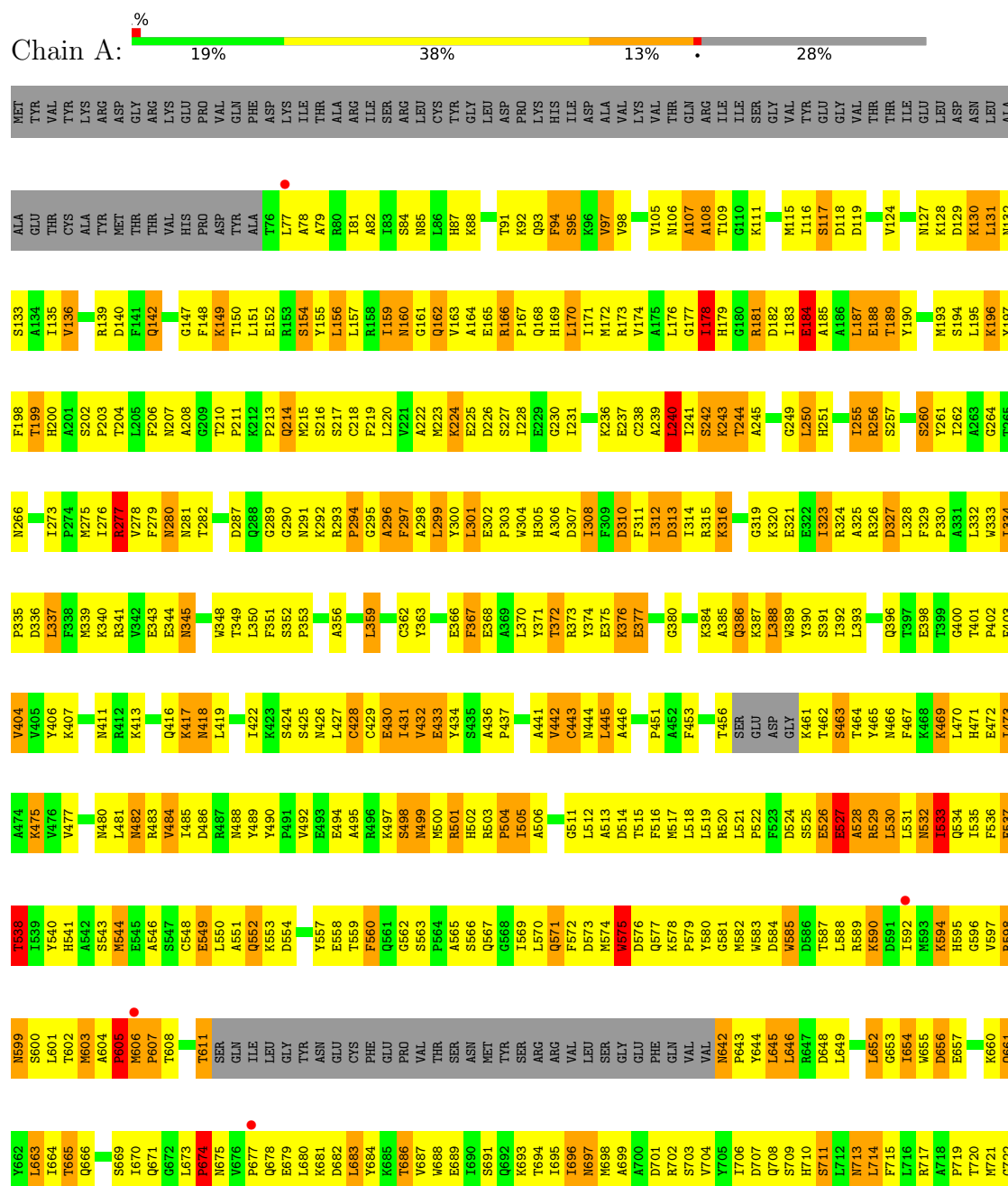


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Ribonucleoside-diphosphate reductase large chain 1



PRO	TYR	SER	K723
ALA	TYR	ALA	L724
PRO	ALA	ALA	L725
THR	THR	ALA	L726
LYS	SER	SER	L727
ASN	ASP	ASP	L728
GLU	PHE	PHE	L729
GLU	VAL	VAL	L730
LYS	PRO	PRO	L731
ALA	ALA	ALA	L732
ALA	ALA	ALA	L733
PRO	VAL	VAL	L734
ILE	THR	THR	L735
VAL	ALA	ALA	L736
ASP	ASN	ASN	L737
ASP	ALA	ALA	L738
ASP	THR	THR	L739
GLU	ILE	ILE	L740
GLU	PRO	PRO	L741
THR	SER	SER	L742
PHE	LEU	LEU	L743
ASP	ASP	ASP	L744
ILE	SER	SER	L745
TYR	SER	SER	L746
ASN	SER	SER	L747
LYS	GLU	GLU	L748
SER	ALA	ALA	L749
VAL	SER	SER	L750
ILE	ARG	ARG	L751
ALA	GLU	GLU	L752
CYS	ALA	ALA	L753
ALA	SER	SER	L754
ILE	PRO	PRO	L755
ASP	ALA	ALA	L756
ASN	PRO	PRO	L757
PRO	THR	THR	L758
GLU	GLY	GLY	L759
ALA	SER	SER	L760
CYS	HIS	HIS	L761
GLU	SER	SER	L762
MET	LEU	LEU	L763
CYS	THR	THR	L764
SER	LYS	LYS	L765
GLY	GLY	GLY	L766
	VAL	VAL	L767
	MET	MET	L768
	ALA	ALA	L769
	GLU	GLU	L770
	LEU	LEU	L771
	ASN	ASN	L772
	VAL	VAL	L773
	GLN	GLN	L774
	GLU	GLU	L775
	ARG	ARG	L776
	LYS	LYS	L777
	SER	SER	L778
	PRO	PRO	L779
	TYR	TYR	L780
	GLU	GLU	L781
	VAL	VAL	L782
	PRO	PRO	L783
	GLU	GLU	L784
	VAL	VAL	L785
	ALA	ALA	L786

4 Data and refinement statistics

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 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.9 (50.00-3.20) 91.9 (50.00-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.06 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, R_{free}	0.226 , 0.298 0.226 , 0.296	Depositor DCC
R_{free} test set	656 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.07	1/5210 (0.0%)	1.31	42/7050 (0.6%)

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	477	VAL	CA-C	-5.17	1.46	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	CYS	N-CA-C	-9.00	96.56	109.96
1	A	528	ALA	N-CA-C	-8.45	101.84	112.90
1	A	463	SER	N-CA-C	8.09	120.67	109.18
1	A	178	ILE	N-CA-C	7.88	117.94	110.53
1	A	189	THR	N-CA-C	-7.28	103.50	112.38
1	A	656	ASP	N-CA-C	7.28	126.30	110.80
1	A	575	TRP	CA-C-N	-6.98	112.77	123.17
1	A	575	TRP	C-N-CA	-6.98	112.77	123.17
1	A	552	GLN	CB-CG-CD	6.71	124.01	112.60
1	A	490	TYR	N-CA-C	6.50	118.27	109.24
1	A	442	VAL	N-CA-C	6.29	118.94	109.20
1	A	711	SER	N-CA-C	6.11	119.36	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	GLU	N-CA-C	-5.94	104.50	110.97
1	A	225	GLU	N-CA-C	5.92	117.25	108.60
1	A	297	PHE	N-CA-C	-5.91	100.03	109.96
1	A	562	GLY	N-CA-C	-5.88	107.64	115.40
1	A	606	MET	N-CA-C	5.87	122.78	109.81
1	A	444	ASN	N-CA-C	-5.85	99.20	108.73
1	A	677	PRO	N-CA-C	5.73	120.22	111.11
1	A	310	ASP	N-CA-C	-5.72	105.18	111.82
1	A	367	PHE	N-CA-C	5.61	117.48	111.36
1	A	334	ILE	CB-CA-C	-5.53	104.42	110.78
1	A	261	TYR	N-CA-C	5.48	117.46	108.52
1	A	334	ILE	N-CA-C	5.42	113.85	107.77
1	A	603	MET	N-CA-C	5.35	118.17	109.24
1	A	576	ASP	N-CA-C	5.33	120.02	111.81
1	A	404	VAL	N-CA-C	5.25	115.42	107.75
1	A	327	ASP	N-CA-C	5.24	120.83	113.02
1	A	648	ASP	N-CA-C	5.21	118.42	111.75
1	A	166	ARG	N-CA-C	-5.20	103.49	109.93
1	A	729	PHE	N-CA-C	-5.19	106.10	112.90
1	A	730	TYR	CA-C-N	5.17	125.82	120.03
1	A	730	TYR	C-N-CA	5.17	125.82	120.03
1	A	411	ASN	CA-C-N	5.17	127.52	120.54
1	A	411	ASN	C-N-CA	5.17	127.52	120.54
1	A	733	LYS	N-CA-C	-5.11	105.83	111.71
1	A	163	VAL	N-CA-C	5.10	114.95	108.12
1	A	277	ARG	N-CA-C	-5.08	106.18	112.38
1	A	578	LYS	N-CA-C	-5.07	103.31	110.31
1	A	504	PRO	CB-CA-C	-5.06	105.26	111.64
1	A	538	THR	N-CA-C	5.04	116.86	111.36
1	A	359	LEU	N-CA-C	5.01	116.82	111.36

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	525	0
2	A	1	0	0	0	0
3	A	31	0	13	6	0
All	All	5126	0	5068	527	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 52.

All (527) 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
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:693:LYS:HE2	1:A:727:MET:HE1	1.40	1.03
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: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:571:GLN:HA	1:A:571:GLN:NE2	1.67	0.98
1:A:181:ARG:HG2	1:A:181:ARG:HH11	1.27	0.97
1:A:417:LYS:HE3	1:A:574:MET:HE1	1.45	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:237:GLU:C	1:A:239:ALA:H	1.89	0.80
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:720:THR:C	1:A:722:GLY:H	1.88	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
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:N	1:A:418:ASN:HD22	1.81	0.77
1:A:224:LYS:HA	1:A:437:PRO:HB3	1.67	0.77
1:A:181:ARG:HG2	1:A:181:ARG:NH1	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:77:LEU:HG	1:A:78:ALA:H	1.50	0.76
1:A:255:ILE:HD12	1:A:275:MET:SD	2.26	0.76
1:A:575:TRP:CZ2	1:A:703:SER:HB3	2.21	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: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:106:ASN:OD1	1:A:109:THR:HG23	1.86	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:SER:OG	1:A:710:HIS:N	2.20	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:193:MET:HE3	1:A:199:THR:HA	1.70	0.73
1:A:280:ASN:CB	1:A:328:LEU:HD11	2.12	0.73
1:A:475:LYS:HG2	1:A:546:ALA:HB2	1.71	0.72
1:A:709:SER:OG	1:A:738:THR:OG1	1.81	0.72
1:A:256:ARG:HA	1:A:353:PRO:HD2	1.69	0.72
1:A:289:GLY:C	1:A:291:ASN:H	1.94	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:661:GLN:HA	1:A:661:GLN:NE2	2.05	0.71
1:A:740:MET:SD	1:A:742:TYR:N	2.64	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:504:PRO:C	1:A:505:ILE:HD13	2.17	0.69
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:HE2	1:A:590:LYS:O	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:207:ASN:ND2	1:A:214:GLN:O	2.25	0.67
1:A:709:SER:HG	1:A:738:THR:HG1	0.85	0.67
1:A:214:GLN:HE21	1:A:245:ALA:HA	1.60	0.67
1:A:277:ARG:CG	1:A:323:ILE:HD13	2.24	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:131:LEU:HG	1:A:172:MET:HE2	1.76	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:91:THR:HG23	1:A:97:VAL:HG22	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:MET:SD	1:A:740:MET:C	2.79	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:693:LYS:HE2	1:A:727:MET:CE	2.23	0.65
1:A:693:LYS:CE	1:A:727:MET:HE1	2.22	0.65
3:A:890:ANP:O1A	3:A:890:ANP:C8	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:720:THR:C	1:A:722:GLY:N	2.51	0.63
1:A:167:PRO:O	1:A:171:ILE:HG13	1.99	0.62
1:A:607:PRO:HD2	1:A:608:THR:HG23	1.80	0.62
1:A:577:GLN:NE2	1:A:704:VAL:HG11	2.15	0.62
1:A:714:LEU:HD13	1:A:740:MET:HG2	1.81	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:HD13	1:A:505:ILE:N	2.14	0.61
1:A:183:ILE:HG22	1:A:187:LEU:HD12	1.83	0.61
1:A:574:MET:C	1:A:575:TRP:O	2.40	0.61
1:A:605:PRO:O	1:A:607:PRO:HD3	2.01	0.61
1:A:151:LEU:HD23	1:A:155:TYR:HB2	1.81	0.61
1:A:182:ASP:CG	1:A:483:ARG:HH22	2.09	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:289:GLY:C	1:A:291:ASN:N	2.60	0.60
1:A:446:ALA:N	1:A:481:LEU:HD11	2.17	0.60
1:A:334:ILE:HD12	1:A:404:VAL:HG13	1.83	0.60
1:A:642:ASN:HB2	1:A:645:LEU:HD23	1.82	0.60
1:A:139:ARG:HD3	1:A:194:SER:HB2	1.83	0.60
1:A:367:PHE:CD1	1:A:367:PHE:C	2.80	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:532:ASN:O	1:A:533:ILE:C	2.43	0.59
1:A:714:LEU:HD11	1:A:740:MET:HG2	1.84	0.59
1:A:257:SER:O	1:A:260:SER:HB2	2.03	0.59
1:A:663:LEU:O	1:A:664:ILE:C	2.45	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:98:VAL:HG21	1:A:124:VAL:HG11	1.84	0.58
1:A:184:GLU:HG3	1:A:185:ALA:H	1.69	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:497:LYS:HG3	1:A:501:ARG:HD3	1.86	0.58
1:A:594:LYS:HD3	1:A:595:HIS:CD2	2.37	0.58
1:A:649:LEU:HB2	1:A:655:TRP:CZ2	2.39	0.58
1:A:135:ILE:HD11	1:A:172:MET:HG2	1.86	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:325:ALA:HB1	1:A:328:LEU:HD12	1.84	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:654:ILE:O	1:A:655:TRP:CG	2.57	0.58
1:A:686:THR:HG23	1:A:688:TRP:CD1	2.38	0.58
1:A:304:TRP:CE3	1:A:304:TRP:C	2.82	0.58
1:A:502:HIS:C	1:A:504:PRO:HD3	2.28	0.58
1:A:255:ILE:CD1	1:A:275:MET:SD	2.91	0.58
1:A:513:ALA:O	1:A:517:MET:HE2	2.04	0.57
1:A:136:VAL:HG22	1:A:136:VAL:O	2.03	0.57
1:A:645:LEU:O	1:A:646:LEU:C	2.47	0.57
1:A:227:SER:HA	3:A:890:ANP:H5'1	1.86	0.57
1:A:417:LYS:CE	1:A:574:MET:HE1	2.28	0.57
1:A:325:ALA:O	1:A:327:ASP:N	2.37	0.57
1:A:213:PRO:HD2	1:A:489:TYR:HB2	1.87	0.57
1:A:373:ARG:HA	1:A:376:LYS:HB2	1.86	0.57
1:A:524:ASP:O	1:A:525:SER:C	2.47	0.57
1:A:106:ASN:OD1	1:A:109:THR:N	2.38	0.57
1:A:525:SER:OG	1:A:528:ALA:HB2	2.05	0.57
1:A:139:ARG:HA	1:A:142:GLN:HG2	1.87	0.57
1:A:200:HIS:CE1	1:A:480:ASN:HB3	2.40	0.57
1:A:154:SER:O	1:A:206:PHE:HE2	1.89	0.56
1:A:297:PHE:HB3	1:A:328:LEU:HD23	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:PHE:O	1:A:537:GLU:C	2.47	0.56
1:A:548:CYS:HG	1:A:552:GLN:CD	2.12	0.56
1:A:445:LEU:HB3	1:A:506:ALA:HB3	1.87	0.56
1:A:362:CYS:HB3	1:A:366:GLU:HG2	1.87	0.56
1:A:107:ALA:O	1:A:108:ALA:HB2	2.05	0.56
1:A:579:PRO:C	1:A:581:GLY:H	2.14	0.56
1:A:570:LEU:H	1:A:573:ASP:HB2	1.71	0.55
1:A:518:LEU:C	1:A:520:ARG:H	2.14	0.55
1:A:551:ALA:HB2	1:A:597:VAL:C	2.32	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:301:LEU:HD12	1:A:311:PHE:CD1	2.41	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:430:GLU:OE2	1:A:607:PRO:HG2	2.06	0.55
1:A:673:LEU:O	1:A:674:PRO:C	2.49	0.55
1:A:84:SER:HA	1:A:87:HIS:HB2	1.88	0.55
1:A:136:VAL:O	1:A:136:VAL:CG2	2.54	0.55
1:A:548:CYS:O	1:A:552:GLN:N	2.34	0.55
1:A:106:ASN:HB3	1:A:111:LYS:H	1.72	0.55
1:A:93:GLN:O	1:A:94:PHE:C	2.49	0.54
1:A:187:LEU:O	1:A:190:TYR:HB3	2.06	0.54
1:A:552:GLN:HG2	1:A:595:HIS:CB	2.37	0.54
1:A:571:GLN:NE2	1:A:571:GLN:CA	2.49	0.54
1:A:94:PHE:CE1	1:A:172:MET:HB3	2.42	0.54
1:A:680:LEU:O	1:A:682:ASP:N	2.40	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:605:PRO:C	1:A:607:PRO:HD3	2.33	0.54
1:A:699:ALA:CA	1:A:702:ARG:HH12	2.17	0.54
1:A:170:LEU:CD1	1:A:170:LEU:C	2.80	0.54
1:A:251:HIS:HB3	1:A:424:SER:HB3	1.90	0.54
1:A:400:GLY:C	1:A:401:THR:HG23	2.31	0.54
1:A:663:LEU:HD11	1:A:670:ILE:CG2	2.38	0.54
1:A:157:LEU:N	1:A:165:GLU:OE1	2.28	0.53
1:A:181:ARG:CG	1:A:181:ARG:NH1	2.54	0.53
1:A:396:GLN:HA	1:A:401:THR:H	1.73	0.53
1:A:442:VAL:HG12	1:A:443:CYS:N	2.23	0.53
1:A:214:GLN:NE2	1:A:245:ALA:HA	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:VAL:HG22	1:A:432:VAL:O	2.07	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: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:384:LYS:O	1:A:387:LYS:N	2.27	0.53
1:A:470:LEU:O	1:A:471:HIS:C	2.52	0.53
1:A:548:CYS:SG	1:A:552:GLN:OE1	2.52	0.53
1:A:308:ILE:O	1:A:312:ILE:HG12	2.09	0.53
1:A:429:CYS:O	1:A:738:THR:CG2	2.57	0.53
1:A:518:LEU:C	1:A:520:ARG:N	2.67	0.53
1:A:686:THR:HG22	1:A:689:GLU:H	1.74	0.53
1:A:257:SER:HA	1:A:307:ASP:OD2	2.08	0.52
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: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:680:LEU:C	1:A:682:ASP:H	2.18	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:117:SER:O	1:A:118:ASP:C	2.52	0.52
1:A:548:CYS:O	1:A:549:GLU:C	2.52	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: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:514:ASP:O	1:A:515:THR:C	2.51	0.51
1:A:588:LEU:C	1:A:590:LYS:N	2.68	0.51
1:A:106:ASN:CG	1:A:109:THR:HG23	2.34	0.51
1:A:182:ASP:OD1	1:A:185:ALA:CB	2.58	0.51
1:A:526:GLU:HA	1:A:529:ARG:HB2	1.93	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:713:ASN:HA	1:A:742:TYR:O	2.10	0.51
1:A:179:HIS:HD2	1:A:483:ARG:CZ	2.23	0.51
1:A:213:PRO:O	1:A:215:MET:HE2	2.11	0.51
1:A:220:LEU:HD22	1:A:425:SER:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLU:O	1:A:345:ASN:C	2.54	0.51
1:A:653:GLY:O	1:A:654:ILE:HB	2.10	0.51
1:A:273:ILE:HG13	1:A:310:ASP:HB3	1.92	0.51
1:A:486:ASP:OD2	1:A:503:ARG:NH2	2.43	0.51
1:A:701:ASP:O	1:A:704:VAL:HG22	2.10	0.51
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:170:LEU:HD13	1:A:174:VAL:HG23	1.93	0.50
1:A:216:SER:HB3	1:A:442:VAL:CG1	2.42	0.50
1:A:334:ILE:CD1	1:A:404:VAL:HG13	2.42	0.50
1:A:719:PRO:HB2	1:A:724:LEU:HD21	1.93	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:257:SER:CB	1:A:306:ALA:HB3	2.42	0.50
1:A:467:PHE:CE1	1:A:582:MET:HE1	2.47	0.50
1:A:538:THR:HB	1:A:583:TRP:NE1	2.27	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:695:ILE:O	1:A:696:ILE:C	2.54	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:130:LYS:NZ	1:A:130:LYS:CB	2.76	0.49
1:A:202:SER:HB3	1:A:206:PHE:CE1	2.48	0.49
1:A:540:TYR:O	1:A:544:MET:HB2	2.13	0.49
1:A:241:ILE:C	1:A:243:LYS:H	2.20	0.49
1:A:525:SER:C	1:A:527:GLU:H	2.20	0.49
1:A:503:ARG:N	1:A:504:PRO:HD3	2.27	0.49
1:A:600:SER:C	1:A:601:LEU:HD12	2.37	0.49
1:A:202:SER:CB	1:A:203:PRO:HD3	2.35	0.49
1:A:241:ILE:C	1:A:243:LYS:N	2.70	0.49
1:A:262:ILE:HG22	1:A:264:GLY:N	2.17	0.49
1:A:514:ASP:O	1:A:517:MET:N	2.46	0.49
1:A:166:ARG:HD2	1:A:169:HIS:HE1	1.78	0.48
1:A:218:CYS:N	1:A:443:CYS:SG	2.85	0.48
1:A:481:LEU:HB3	1:A:505:ILE:HG23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:THR:O	1:A:208:ALA:CB	2.61	0.48
1:A:560:PHE:O	1:A:563:SER:HB2	2.13	0.48
1:A:226:ASP:OD2	1:A:256:ARG:HG2	2.14	0.48
1:A:530:LEU:O	1:A:531:LEU:C	2.56	0.48
1:A:569:ILE:C	1:A:570:LEU:HD23	2.38	0.48
1:A:686:THR:CG2	1:A:688:TRP:CD1	2.88	0.48
1:A:298:ALA:HB2	1:A:427:LEU:HD13	1.94	0.48
1:A:654:ILE:O	1:A:655:TRP:CD1	2.67	0.48
1:A:714:LEU:HD21	1:A:740:MET:HG3	1.95	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:579:PRO:C	1:A:581:GLY:N	2.72	0.48
1:A:222:ALA:O	1:A:224:LYS:N	2.47	0.48
1:A:238:CYS:SG	1:A:297:PHE:CZ	2.94	0.48
1:A:691:SER:O	1:A:695:ILE:HG13	2.14	0.48
1:A:279:PHE:C	1:A:281:ASN:H	2.22	0.48
1:A:582:MET:O	1:A:582:MET:CG	2.62	0.48
1:A:386:GLN:O	1:A:390:TYR:HB2	2.14	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:350:LEU:O	1:A:380:GLY:HA3	2.14	0.47
1:A:109:THR:OG1	1:A:111:LYS:HG3	2.14	0.47
1:A:304:TRP:C	1:A:304:TRP:HE3	2.21	0.47
1:A:392:ILE:O	1:A:393:LEU:C	2.56	0.47
1:A:535:ILE:O	1:A:538:THR:HG23	2.14	0.47
1:A:400:GLY:C	1:A:401:THR:CG2	2.86	0.47
1:A:431:ILE:HG13	1:A:433:GLU:HG3	1.97	0.47
1:A:738:THR:C	1:A:739:GLY:O	2.56	0.47
1:A:304:TRP:HE3	1:A:304:TRP:O	1.97	0.47
1:A:608:THR:CG2	1:A:611:THR:HG21	2.45	0.47
1:A:130:LYS:C	1:A:133:SER:OG	2.57	0.47
1:A:166:ARG:HD2	1:A:169:HIS:CE1	2.49	0.47
1:A:428:CYS:HB3	1:A:607:PRO:HB2	1.97	0.47
1:A:467:PHE:HE1	1:A:582:MET:HE1	1.79	0.47
1:A:469:LYS:HA	1:A:469:LYS:HD3	1.50	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:713:ASN:O	1:A:715:PHE:CD1	2.67	0.47
1:A:210:THR:CB	1:A:211:PRO:CD	2.91	0.47
1:A:95:SER:OG	1:A:132:ASN:ND2	2.43	0.47
1:A:230:GLY:O	1:A:231:ILE:C	2.58	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:THR:HG22	1:A:373:ARG:N	2.29	0.47
1:A:557:TYR:HE1	1:A:559:THR:HG23	1.80	0.47
1:A:560:PHE:O	1:A:563:SER:HB3	2.15	0.47
1:A:695:ILE:C	1:A:697:ASN:N	2.70	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:697:ASN:O	1:A:698:MET:C	2.57	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:85:ASN:OD1	1:A:88:LYS:HD2	2.16	0.46
1:A:516:PHE:CE2	1:A:698:MET:HE1	2.51	0.46
1:A:188:GLU:C	1:A:190:TYR:N	2.69	0.46
1:A:344:GLU:O	1:A:344:GLU:HG3	2.15	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:176:LEU:O	1:A:177:GLY:C	2.59	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:198:PHE:CD2	1:A:198:PHE:C	2.94	0.45
1:A:403:PHE:CD1	1:A:741:TYR:HE1	2.34	0.45
1:A:565:ALA:C	1:A:567:GLN:N	2.72	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:588:LEU:C	1:A:590:LYS:H	2.23	0.45
1:A:222:ALA:HA	1:A:251:HIS:CE1	2.51	0.45
1:A:339:MET:HE2	1:A:406:TYR:CE2	2.51	0.45
1:A:403:PHE:CD1	1:A:741:TYR:CE1	3.05	0.45
1:A:494:GLU:O	1:A:495:ALA:C	2.58	0.45
1:A:517:MET:HE3	1:A:517:MET:HB2	1.85	0.45
1:A:664:ILE:HD12	1:A:665:THR:N	2.30	0.45
1:A:375:GLU:O	1:A:376:LYS:C	2.60	0.45
1:A:467:PHE:CD1	1:A:582:MET:SD	3.10	0.45
1:A:498:SER:O	1:A:500:MET:N	2.49	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:740:MET:SD	1:A:742:TYR:C	2.99	0.45
1:A:127:ASN:O	1:A:128:LYS:C	2.59	0.45
1:A:579:PRO:HB2	1:A:581:GLY:H	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:GLN:HE21	1:A:669:SER:HB3	1.82	0.45
1:A:605:PRO:HG2	1:A:706:ILE:CD1	2.47	0.45
1:A:219:PHE:CE1	1:A:245:ALA:HB1	2.51	0.45
1:A:323:ILE:HG22	1:A:325:ALA:CA	2.46	0.45
1:A:549:GLU:O	1:A:553:LYS:N	2.37	0.45
1:A:178:ILE:HG22	1:A:483:ARG:HB2	1.98	0.44
1:A:240:LEU:HD23	1:A:240:LEU:HA	1.65	0.44
1:A:696:ILE:HD11	1:A:714:LEU:HD12	1.99	0.44
1:A:147:GLY:O	1:A:150:THR:HB	2.16	0.44
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:686:THR:HB	1:A:689:GLU:CD	2.40	0.44
1:A:340:LYS:O	1:A:341:ARG:C	2.60	0.44
1:A:356:ALA:HB1	1:A:374:TYR:CD1	2.52	0.44
1:A:501:ARG:HB3	1:A:501:ARG:NH1	2.33	0.44
1:A:525:SER:OG	1:A:528:ALA:CB	2.65	0.44
1:A:548:CYS:C	1:A:552:GLN:HG3	2.42	0.44
1:A:166:ARG:HB2	1:A:169:HIS:ND1	2.33	0.44
1:A:226:ASP:C	3:A:890:ANP:H5'1	2.41	0.44
1:A:313:ASP:CG	1:A:316:LYS:HG3	2.42	0.44
1:A:654:ILE:O	1:A:655:TRP:CB	2.64	0.44
1:A:678:GLN:O	1:A:679:GLU:C	2.60	0.44
1:A:325:ALA:C	1:A:327:ASP:N	2.76	0.44
1:A:156:LEU:HG	1:A:165:GLU:O	2.17	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:580:TYR:HE1	1:A:582:MET:HE3	1.82	0.44
1:A:697:ASN:C	1:A:699:ALA:N	2.76	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:127:ASN:O	1:A:129:ASP:N	2.51	0.43
1:A:400:GLY:O	1:A:401:THR:HG22	2.18	0.43
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:663:LEU:O	1:A:666:GLN:O	2.36	0.43
1:A:189:THR:O	1:A:193:MET:HG3	2.18	0.43
1:A:195:LEU:O	1:A:197:TYR:N	2.51	0.43
1:A:214:GLN:HE21	1:A:245:ALA:CA	2.30	0.43
1:A:315:ARG:NH1	1:A:328:LEU:O	2.51	0.43
1:A:605:PRO:HD2	1:A:710:HIS:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ARG:HA	1:A:181:ARG:HD3	1.82	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:551:ALA:HB2	1:A:598:ARG:N	2.33	0.43
1:A:251:HIS:CD2	1:A:251:HIS:O	2.72	0.43
1:A:696:ILE:O	1:A:699:ALA:HB3	2.18	0.43
1:A:352:SER:HA	1:A:353:PRO:HD3	1.76	0.43
1:A:305:HIS:O	1:A:308:ILE:HB	2.19	0.43
1:A:336:ASP:O	1:A:337:LEU:C	2.61	0.43
1:A:388:LEU:O	1:A:389:TRP:C	2.61	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:329:PHE:HA	1:A:330:PRO:HD3	1.85	0.43
1:A:466:ASN:OD1	1:A:466:ASN:C	2.62	0.43
1:A:332:LEU:CD1	1:A:392:ILE:HD13	2.49	0.42
1:A:436:ALA:HB1	1:A:437:PRO:HD2	2.01	0.42
1:A:470:LEU:C	1:A:472:GLU:N	2.74	0.42
1:A:688:TRP:CD1	1:A:688:TRP:H	2.37	0.42
1:A:237:GLU:HG2	1:A:492:VAL:HG11	2.02	0.42
1:A:480:ASN:O	1:A:481:LEU:C	2.62	0.42
1:A:485:ILE:HD11	1:A:505:ILE:CD1	2.49	0.42
1:A:565:ALA:C	1:A:567:GLN:H	2.27	0.42
1:A:81:ILE:HD12	1:A:82:ALA:N	2.35	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:691:SER:O	1:A:694:THR:OG1	2.31	0.42
1:A:296:ALA:HB1	1:A:427:LEU:HD22	1.97	0.42
1:A:588:LEU:O	1:A:590:LYS:N	2.53	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:652:LEU:H	1:A:652:LEU:HG	1.58	0.42
1:A:572:PHE:CD2	1:A:579:PRO:HD3	2.55	0.42
1:A:339:MET:SD	1:A:389:TRP:HZ3	2.43	0.42
1:A:588:LEU:HD12	1:A:588:LEU:HA	1.86	0.42
1:A:713:ASN:O	1:A:715:PHE:HD1	2.03	0.42
1:A:335:PRO:HB3	1:A:407:LYS:HD3	2.02	0.41
1:A:453:PHE:HB2	1:A:465:TYR:CE2	2.55	0.41
1:A:472:GLU:O	1:A:473:ILE:C	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PHE:CZ	1:A:172:MET:HG3	2.55	0.41
1:A:280:ASN:O	1:A:280:ASN:CG	2.62	0.41
1:A:325:ALA:CB	1:A:328:LEU:HD12	2.49	0.41
1:A:148:PHE:O	1:A:149:LYS:C	2.63	0.41
1:A:453:PHE:HB2	1:A:465:TYR:CZ	2.55	0.41
1:A:219:PHE:HA	1:A:441:ALA:O	2.20	0.41
1:A:308:ILE:HD11	1:A:332:LEU:CD2	2.50	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:725:THR:O	1:A:729:PHE:HD1	2.03	0.41
1:A:740:MET:SD	1:A:741:TYR:N	2.93	0.41
1:A:91:THR:CG2	1:A:97:VAL:HG22	2.50	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:693:LYS:O	1:A:697:ASN:HB2	2.20	0.41
1:A:92:LYS:HA	1:A:166:ARG:NH2	2.36	0.41
1:A:94:PHE:HD1	1:A:169:HIS:CD2	2.38	0.41
1:A:575:TRP:CD1	1:A:704:VAL:HA	2.55	0.41
1:A:671:GLN:HG2	1:A:689:GLU:OE2	2.20	0.41
1:A:714:LEU:HD11	1:A:740:MET:CG	2.48	0.41
1:A:85:ASN:HA	1:A:88:LYS:HD2	2.03	0.41
1:A:107:ALA:O	1:A:108:ALA:CB	2.68	0.41
1:A:130:LYS:O	1:A:133:SER:OG	2.39	0.41
1:A:170:LEU:HD22	1:A:173:ARG:HH21	1.85	0.41
1:A:202:SER:CB	1:A:203:PRO:CD	2.88	0.41
1:A:343:GLU:OE2	1:A:733:LYS:HE3	2.21	0.41
1:A:363:TYR:CA	1:A:367:PHE:HB2	2.48	0.41
1:A:541:HIS:NE2	1:A:588:LEU:HD22	2.35	0.41
1:A:602:THR:N	1:A:707:ASP:OD2	2.54	0.41
1:A:160:ASN:C	1:A:162:GLN:H	2.29	0.41
1:A:296:ALA:HB1	1:A:427:LEU:HD21	1.97	0.41
1:A:300:TYR:OH	1:A:429:CYS:SG	2.71	0.41
1:A:384:LYS:O	1:A:385:ALA:C	2.63	0.41
1:A:413:LYS:NZ	1:A:735:GLY:O	2.53	0.41
1:A:536:PHE:N	1:A:536:PHE:CD2	2.89	0.41
1:A:552:GLN:CG	1:A:595:HIS:ND1	2.81	0.41
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.55	0.41
1:A:649:LEU:HB2	1:A:655:TRP:CE2	2.56	0.41
1:A:183:ILE:CG2	1:A:187:LEU:CD1	2.99	0.40
1:A:308:ILE:HG21	1:A:388:LEU:HD11	2.03	0.40
1:A:467:PHE:HD1	1:A:582:MET:SD	2.44	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:213:PRO:CD	1:A:489:TYR:HB2	2.52	0.40
1:A:312:ILE:HD13	1:A:312:ILE:HG21	1.87	0.40
1:A:429:CYS:HB3	1:A:738:THR:HG23	2.03	0.40
1:A:642:ASN:HA	1:A:643:PRO:HD3	1.92	0.40
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.81	0.40
1:A:534:GLN:O	1:A:537:GLU:HB3	2.20	0.40
1:A:293:ARG:N	1:A:294:PRO:HD2	2.36	0.40
1:A:305:HIS:ND1	1:A:307:ASP:HB2	2.36	0.40
1:A:518:LEU:HD21	1:A:644:TYR:OH	2.21	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 7

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	674	PRO
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 ⓘ

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	550/761 (72%)	430 (78%)	120 (22%)	1 6

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	SER
1	A	97	VAL
1	A	115	MET
1	A	116	ILE
1	A	117	SER
1	A	130	LYS
1	A	131	LEU
1	A	136	VAL
1	A	142	GLN
1	A	149	LYS
1	A	152	GLU
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	196	LYS
1	A	199	THR
1	A	214	GLN
1	A	224	LYS
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	255	ILE
1	A	256	ARG
1	A	260	SER
1	A	266	ASN
1	A	277	ARG
1	A	282	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	287	ASP
1	A	292	LYS
1	A	299	LEU
1	A	301	LEU
1	A	308	ILE
1	A	312	ILE
1	A	313	ASP
1	A	316	LYS
1	A	320	LYS
1	A	323	ILE
1	A	324	ARG
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	391	SER
1	A	398	GLU
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	443	CYS
1	A	445	LEU
1	A	456	THR
1	A	461	LYS
1	A	462	THR
1	A	463	SER
1	A	464	THR
1	A	469	LYS
1	A	473	ILE
1	A	475	LYS
1	A	482	ASN
1	A	501	ARG
1	A	505	ILE
1	A	512	LEU
1	A	526	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	527	GLU
1	A	529	ARG
1	A	530	LEU
1	A	533	ILE
1	A	537	GLU
1	A	538	THR
1	A	543	SER
1	A	544	MET
1	A	549	GLU
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	592	ILE
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	683	LEU
1	A	686	THR
1	A	687	VAL
1	A	696	ILE
1	A	697	ASN
1	A	711	SER
1	A	713	ASN
1	A	714	LEU
1	A	723	LYS
1	A	726	SER
1	A	743	LEU
1	A	746	GLN

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

Mol	Chain	Res	Type
1	A	179	HIS
1	A	200	HIS
1	A	251	HIS
1	A	280	ASN
1	A	291	ASN
1	A	345	ASN
1	A	386	GLN
1	A	416	GLN
1	A	418	ASN
1	A	444	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
1	A	728	HIS

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 oligosaccharides 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	33,33,33	1.82	7 (21%)	45,52,52	2.60	15 (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	-	1/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	890	ANP	C5-C4	4.94	1.47	1.39
3	A	890	ANP	PB-O1B	4.21	1.52	1.46
3	A	890	ANP	PG-O1G	3.64	1.51	1.46
3	A	890	ANP	C5-N7	-3.37	1.32	1.39
3	A	890	ANP	PB-O3A	2.42	1.62	1.59
3	A	890	ANP	C4-N9	-2.30	1.32	1.37
3	A	890	ANP	C8-N7	2.02	1.35	1.31

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	890	ANP	O1G-PG-N3B	-10.74	95.96	111.77
3	A	890	ANP	C5-C4-N3	-4.71	120.23	126.72
3	A	890	ANP	O2B-PB-O1B	4.16	118.79	109.87
3	A	890	ANP	O4'-C1'-N9	4.15	116.06	108.09
3	A	890	ANP	O1B-PB-N3B	-4.14	105.68	111.77
3	A	890	ANP	N3-C4-N9	4.06	134.07	127.17
3	A	890	ANP	O2G-PG-O3G	3.82	117.85	107.59
3	A	890	ANP	N3-C2-N1	-3.56	123.20	128.58
3	A	890	ANP	C2-N3-C4	2.96	119.06	111.83
3	A	890	ANP	C2-N1-C6	2.86	123.43	118.73
3	A	890	ANP	C3'-C2'-C1'	2.84	106.84	101.46
3	A	890	ANP	N6-C6-N1	2.72	124.44	118.38
3	A	890	ANP	O2B-PB-O3A	2.65	113.47	104.64
3	A	890	ANP	O2'-C2'-C1'	-2.36	101.98	110.10
3	A	890	ANP	O3A-PB-N3B	-2.04	100.93	106.59

There are no chirality outliers.

All (1) torsion outliers are listed below:

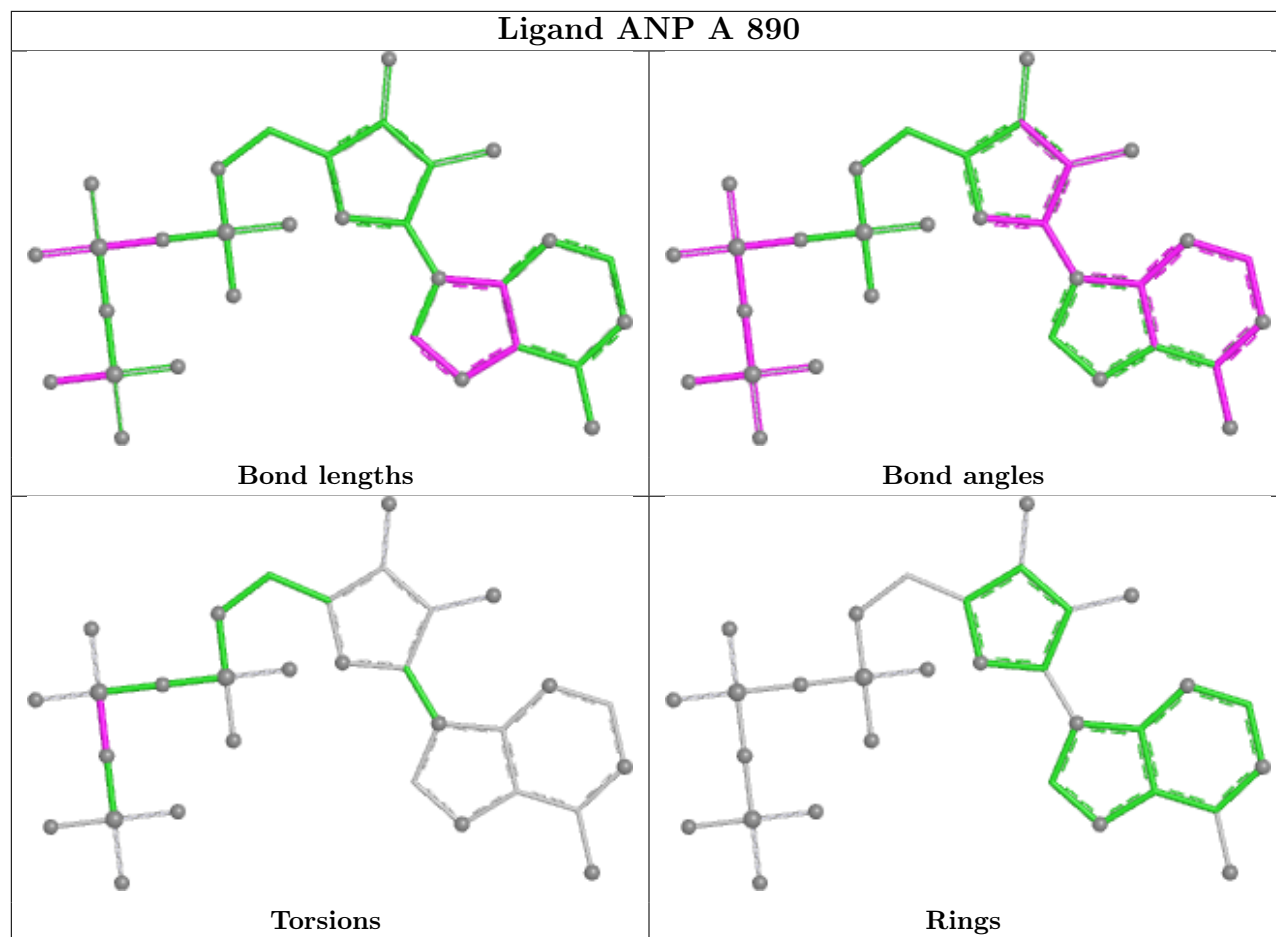
Mol	Chain	Res	Type	Atoms
3	A	890	ANP	PG-N3B-PB-O3A

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	890	ANP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	637/888 (71%)	-0.19	5 (0%) 82 67	54, 78, 129, 154	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	592	ILE	3.1
1	A	77	LEU	2.8
1	A	606	MET	2.4
1	A	677	PRO	2.4
1	A	741	TYR	2.2

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](#)

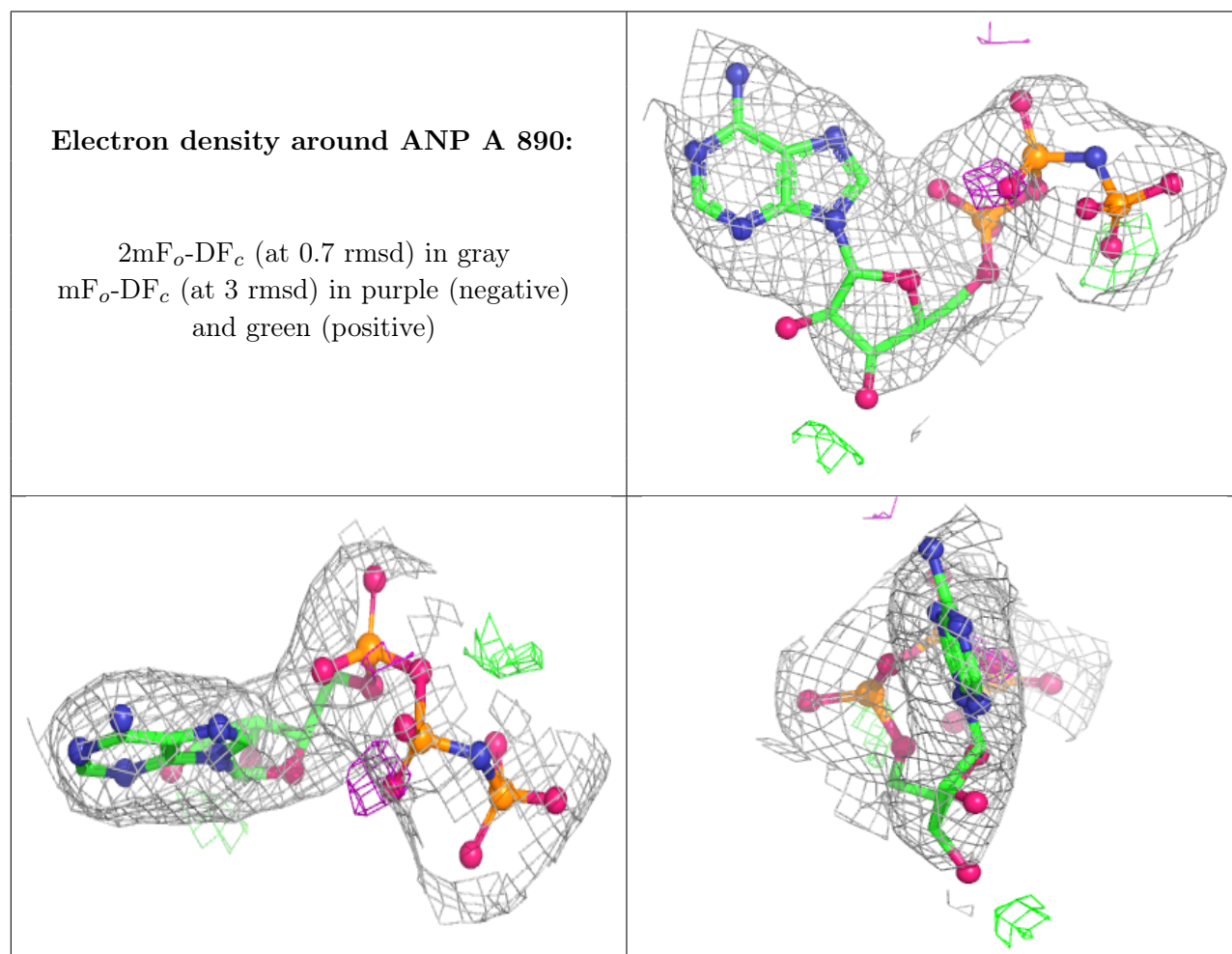
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
2	MG	A	889	1/1	0.81	0.19	67,67,67,67	0
3	ANP	A	890	31/31	0.92	0.08	83,87,101,103	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.