



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:59 AM GMT

PDB ID : 2OZO  
Title : Autoinhibited intact human ZAP-70  
Authors : Deindl, S.; Kadlecsek, T.A.; Brdicka, T.; Cao, X.; Weiss, A.; Kuriyan, J.  
Deposited on : 2007-02-26  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

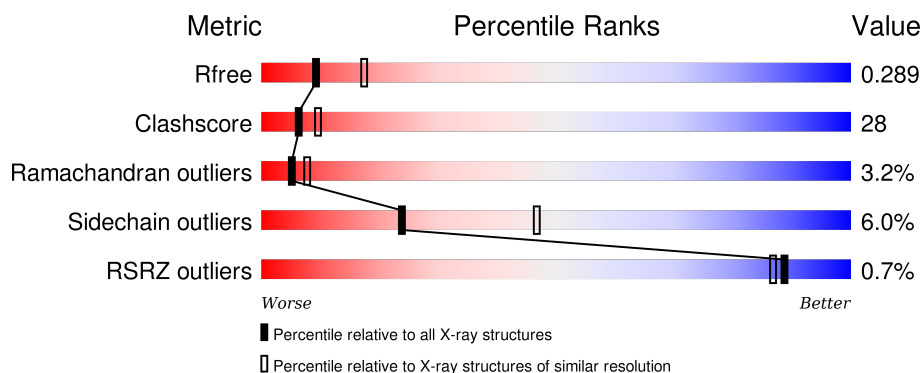
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	613	<div> <div></div> <div>48%</div> <div>37%</div> <div>•</div> <div>11%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4326 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 Tyrosine-protein kinase ZAP-70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4225	2705	727	759	34			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	PHE	TYR	ENGINEERED	UNP P43403
A	319	PHE	TYR	ENGINEERED	UNP P43403
A	461	ASN	ASP	ENGINEERED	UNP P43403
A	607	GLY	-	CLONING ARTIFACT	UNP P43403
A	608	SER	-	CLONING ARTIFACT	UNP P43403
A	609	ALA	-	CLONING ARTIFACT	UNP P43403
A	610	LEU	-	CLONING ARTIFACT	UNP P43403
A	611	GLU	-	CLONING ARTIFACT	UNP P43403
A	612	VAL	-	CLONING ARTIFACT	UNP P43403
A	613	ALA	-	CLONING ARTIFACT	UNP P43403

- 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<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	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	69	Total	0	0
			69 O		

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 ( $\text{RSRZ} > 2$ ). 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.

Chain A: ● ■ 48% ■ 37% ■ 11%

Residue	Category	Percentage
M580	Red	48%
M581	Red	48%
D582	Red	48%
R583	Red	48%
F586	Red	48%
L587	Red	48%
T588	Red	48%
V589	Red	48%
M593	Red	48%
Y597	Red	48%
S602	Red	48%
K603	Red	48%
V604	Red	48%
E605	Red	48%
G606	Red	48%
G607	Red	48%
S608	Red	48%
A609	Red	48%
L610	Red	48%
E611	Red	48%
V612	Red	48%
A613	Red	48%
L503	Green	37%
K504	Green	37%
R505	Green	37%
Y506	Green	37%
E509	Green	37%
R514	Green	37%
R515	Green	37%
F516	Green	37%
S517	Green	37%
S518	Green	37%
R519	Green	37%
S520	Green	37%
D521	Green	37%
V522	Green	37%
K523	Green	37%
S524	Green	37%
V525	Green	37%
G526	Green	37%
S527	Green	37%
V528	Green	37%
M529	Green	37%
K530	Green	37%
E531	Green	37%
A532	Green	37%
L533	Green	37%
Q537	Green	37%
K538	Green	37%
P539	Green	37%
Y540	Green	37%
K544	Green	37%
G545	Green	37%
F551	Green	37%
I552	Green	37%
K556	Green	37%
R557	Green	37%
M558	Green	37%
E559	Green	37%
A560	Green	37%
P561	Green	37%
P562	Green	37%
P565	Green	37%
P566	Green	37%
E567	Green	37%
L568	Green	37%
K572	Green	37%
S573	Green	37%
D574	Green	37%
C575	Green	37%
H576	Green	37%
I577	Green	37%
V578	Green	37%
V579	Green	37%
F331	Yellow	37%
R430	Yellow	37%
E431	Yellow	37%
K432	Yellow	37%
E433	Yellow	37%
R434	Yellow	37%
P434	Yellow	37%
M437	Yellow	37%
E440	Yellow	37%
L441	Yellow	37%
V445	Yellow	37%
S446	Yellow	37%
M447	Yellow	37%
G448	Yellow	37%
M449	Yellow	37%
K450	Yellow	37%
E453	Yellow	37%
E454	Yellow	37%
H459	Yellow	37%
R460	Yellow	37%
M461	Yellow	37%
L462	Yellow	37%
L469	Yellow	37%
V470	Yellow	37%
M471	Yellow	37%
R472	Yellow	37%
H473	Yellow	37%
Y474	Yellow	37%
A475	Yellow	37%
K476	Yellow	37%
I477	Yellow	37%
S478	Yellow	37%
D479	Yellow	37%
F480	Yellow	37%
G481	Yellow	37%
L482	Yellow	37%
S483	Yellow	37%
K484	Yellow	37%
A485	Yellow	37%
L486	Yellow	37%
G487	Yellow	37%
ALA	Yellow	37%
ASP	Yellow	37%
ASP	Yellow	37%
SER	Yellow	37%
SER	Yellow	37%
TTR	Yellow	37%
TTR	Yellow	37%
ALA	Yellow	37%
ARG	Yellow	37%
SER	Yellow	37%
D574	Yellow	37%
C575	Yellow	37%
GLY	Yellow	37%
LVS	Yellow	37%
TSP	Yellow	37%
D502	Yellow	37%
F317	Orange	11%
S317	Orange	11%
F318	Orange	11%
F319	Orange	11%
S320	Orange	11%
D321	Orange	11%
P322	Orange	11%
E323	Orange	11%
E324	Orange	11%
L325	Orange	11%
K326	Orange	11%
D327	Orange	11%
K328	Orange	11%
V427	Orange	11%
G428	Orange	11%
K429	Orange	11%
L246	Orange	11%
C249	Orange	11%
L250	Orange</	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.30Å 52.93Å 69.33Å 105.91° 92.94° 103.72°	Depositor
Resolution (Å)	500.00 – 2.60 49.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.3 (500.00-2.60) 79.8 (49.13-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.220 , 0.290 0.219 , 0.289	Depositor DCC
$R_{free}$ test set	1622 reflections (9.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20533 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.42	0/4328	0.67	1/5855 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	326	LYS	N-CA-C	5.01	124.54	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4225	0	4104	232	0
2	A	1	0	0	0	0
3	A	31	0	13	1	0
4	A	69	0	0	9	0
All	All	4326	0	4117	233	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 28.

All (233) 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:430:ARG:HH12	1:A:562:PRO:HB2	1.17	1.08
1:A:604:VAL:HG23	1:A:605:GLU:H	1.19	1.05
1:A:605:GLU:HB2	1:A:610:LEU:HD22	1.48	0.96
1:A:27:ALA:HB3	1:A:33:LEU:HD21	1.48	0.96
1:A:41:ARG:HH22	1:A:226:GLY:HA3	1.35	0.92
1:A:559:GLU:CD	1:A:559:GLU:H	1.76	0.89
1:A:398:ILE:HD12	1:A:477:ILE:HB	1.56	0.87
1:A:230:ASP:HB2	1:A:234:GLN:HE22	1.38	0.86
1:A:471:ASN:HD22	1:A:471:ASN:C	1.79	0.86
1:A:170:ARG:CZ	1:A:190:ARG:HH22	1.91	0.84
1:A:485:ALA:HA	4:A:664:HOH:O	1.79	0.81
1:A:502:PRO:HD3	4:A:657:HOH:O	1.82	0.79
1:A:604:VAL:HG23	1:A:605:GLU:N	1.96	0.78
1:A:181:ALA:O	1:A:186:LYS:HE2	1.82	0.78
1:A:63:ARG:HH11	1:A:63:ARG:HB3	1.49	0.77
1:A:321:ASP:OD1	1:A:323:GLU:HG2	1.85	0.77
1:A:430:ARG:NH1	1:A:562:PRO:HB2	1.97	0.76
1:A:502:PRO:C	1:A:503:LEU:HD22	2.07	0.75
1:A:97:ASN:HD21	1:A:99:ARG:HE	1.33	0.74
1:A:517:SER:H	1:A:520:SER:HB3	1.51	0.74
1:A:343:GLU:OE1	1:A:351:SER:HB2	1.87	0.73
1:A:450:LYS:O	1:A:454:GLU:HG2	1.87	0.73
1:A:41:ARG:NH1	1:A:41:ARG:HB3	2.06	0.71
1:A:398:ILE:CD1	1:A:477:ILE:HB	2.21	0.71
1:A:231:THR:OG1	1:A:234:GLN:HG3	1.91	0.70
1:A:314:VAL:HG12	1:A:319:PHE:CD1	2.26	0.70
1:A:354:GLN:HG3	1:A:416:MET:CE	2.23	0.68
1:A:479:ASP:HB3	1:A:482:LEU:HD11	1.74	0.68
1:A:318:PRO:HB3	4:A:632:HOH:O	1.92	0.68
1:A:611:GLU:C	1:A:613:ALA:H	1.97	0.68
1:A:610:LEU:C	1:A:612:VAL:H	1.98	0.67
1:A:450:LYS:HE3	1:A:587:LEU:HD12	1.77	0.67
1:A:552:ILE:HG23	1:A:557:ARG:HH12	1.58	0.67
1:A:314:VAL:HG13	1:A:474:TYR:CG	2.29	0.66
1:A:375:THR:CB	1:A:380:THR:HG22	2.25	0.66
1:A:354:GLN:HG2	1:A:355:GLY:N	2.11	0.65
1:A:40:LEU:HD22	1:A:40:LEU:H	1.61	0.65
1:A:220:LYS:HE3	1:A:230:ASP:OD2	1.95	0.65
1:A:170:ARG:HB2	1:A:170:ARG:HH11	1.62	0.65
1:A:342:ILE:HD12	1:A:342:ILE:N	2.11	0.64
1:A:577:ILE:HB	1:A:583:ARG:HG2	1.79	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:VAL:HG12	1:A:319:PHE:HD1	1.61	0.64
1:A:2:PRO:HB3	1:A:119:ARG:NH2	2.12	0.64
1:A:216:ASP:OD2	1:A:228:LYS:HE3	1.98	0.64
1:A:611:GLU:C	1:A:613:ALA:N	2.49	0.64
1:A:316:GLU:HB2	4:A:627:HOH:O	1.97	0.64
1:A:330:LEU:HD22	1:A:404:VAL:HG12	1.79	0.64
1:A:316:GLU:O	1:A:317:SER:HB2	1.97	0.63
1:A:198:TYR:HE1	1:A:221:TYR:HE2	1.47	0.63
1:A:552:ILE:HG23	1:A:557:ARG:NH1	2.13	0.63
1:A:603:LYS:O	1:A:604:VAL:HG22	1.99	0.62
1:A:119:ARG:HD2	1:A:150:GLU:OE1	1.99	0.62
1:A:230:ASP:HB2	1:A:234:GLN:NE2	2.14	0.61
1:A:169:THR:OG1	1:A:172:GLU:HG3	2.01	0.61
1:A:471:ASN:ND2	1:A:473:HIS:H	1.98	0.60
1:A:333:LYS:HB2	1:A:336:ASN:HD22	1.67	0.60
1:A:441:LEU:O	1:A:445:VAL:HG23	2.03	0.59
1:A:349:PHE:CE1	1:A:482:LEU:HD13	2.37	0.59
1:A:97:ASN:ND2	1:A:99:ARG:HE	2.00	0.58
1:A:459:HIS:O	1:A:460:ARG:HB2	2.02	0.58
1:A:529:MET:HB3	1:A:572:MET:HE2	1.84	0.58
1:A:231:THR:N	1:A:234:GLN:HE21	2.02	0.58
1:A:471:ASN:ND2	1:A:471:ASN:C	2.52	0.58
1:A:460:ARG:HG2	1:A:516:PHE:CD2	2.39	0.58
1:A:27:ALA:CB	1:A:33:LEU:HD21	2.29	0.57
1:A:97:ASN:HD22	1:A:97:ASN:H	1.50	0.57
1:A:128:ARG:O	1:A:132:LYS:HA	2.03	0.57
1:A:328:LYS:HG3	1:A:328:LYS:O	2.03	0.57
1:A:33:LEU:HA	1:A:100:LYS:O	2.03	0.57
1:A:223:ILE:CG2	1:A:235:LEU:HD21	2.34	0.57
1:A:369:LYS:NZ	1:A:479:ASP:OD1	2.37	0.57
1:A:518:SER:O	1:A:522:VAL:HG23	2.05	0.56
1:A:604:VAL:CG2	1:A:605:GLU:H	2.04	0.56
1:A:97:ASN:HD21	1:A:99:ARG:NE	2.02	0.56
1:A:517:SER:O	1:A:520:SER:HB3	2.04	0.56
1:A:48:LEU:HB2	1:A:61:ILE:HD11	1.87	0.55
1:A:362:LYS:HD2	1:A:364:ILE:HG22	1.89	0.55
1:A:41:ARG:HB3	1:A:41:ARG:HH11	1.71	0.55
1:A:350:GLY:HA2	1:A:371:LEU:HD23	1.88	0.55
1:A:198:TYR:CE1	1:A:221:TYR:HE2	2.25	0.55
1:A:568:LEU:HD22	1:A:593:MET:CE	2.37	0.55
1:A:161:MET:HG3	1:A:163:TRP:CZ2	2.42	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLY:N	4:A:672:HOH:O	2.39	0.55
1:A:46:TYR:CE2	1:A:80:PRO:HG3	2.42	0.54
1:A:577:ILE:HG21	1:A:582:ASP:HB2	1.88	0.54
1:A:509:GLU:OE2	1:A:580:TRP:HB3	2.07	0.54
1:A:559:GLU:N	1:A:559:GLU:OE2	2.40	0.54
1:A:145:GLN:HG3	1:A:315:PHE:CZ	2.42	0.54
1:A:337:LEU:HD23	1:A:339:ILE:HD11	1.90	0.53
1:A:202:LEU:CD2	1:A:209:TYR:HB2	2.39	0.53
1:A:502:PRO:O	1:A:503:LEU:HD22	2.07	0.53
1:A:574:ASP:O	1:A:577:ILE:HG12	2.07	0.53
1:A:336:ASN:ND2	4:A:681:HOH:O	2.40	0.53
1:A:35:LEU:C	1:A:35:LEU:HD12	2.28	0.53
1:A:460:ARG:O	1:A:506:TYR:HE1	1.91	0.52
1:A:239:LEU:HB2	1:A:250:LEU:HD12	1.92	0.52
1:A:203:ILE:CD1	1:A:208:VAL:HG22	2.39	0.52
1:A:136:GLU:O	1:A:140:GLN:N	2.38	0.52
1:A:314:VAL:HG13	1:A:474:TYR:CD1	2.45	0.51
1:A:482:LEU:HD12	1:A:483:SER:N	2.26	0.51
1:A:173:ALA:O	1:A:177:LEU:HG	2.10	0.51
1:A:334:ARG:HD3	1:A:407:ALA:CB	2.40	0.51
1:A:83:LEU:HD23	1:A:83:LEU:C	2.30	0.51
1:A:322:PRO:HG2	1:A:402:ILE:CD1	2.40	0.51
1:A:559:GLU:CD	1:A:559:GLU:N	2.56	0.51
1:A:440:GLU:HG3	1:A:597:TYR:CZ	2.45	0.51
1:A:97:ASN:N	1:A:97:ASN:HD22	2.08	0.51
1:A:188:LEU:O	1:A:189:LEU:HD12	2.09	0.51
1:A:41:ARG:HH12	1:A:227:THR:N	2.08	0.51
1:A:502:PRO:O	1:A:503:LEU:HD13	2.10	0.50
1:A:544:LYS:HG3	1:A:545:GLY:N	2.26	0.50
1:A:551:PHE:CE1	1:A:556:LYS:HB3	2.46	0.50
1:A:333:LYS:HB2	1:A:336:ASN:ND2	2.25	0.50
1:A:437:ASN:ND2	1:A:472:ARG:HH21	2.09	0.50
1:A:178:TYR:CZ	1:A:208:VAL:HG23	2.45	0.50
1:A:155:THR:O	1:A:155:THR:HG22	2.12	0.50
1:A:170:ARG:HB2	1:A:170:ARG:NH1	2.26	0.50
1:A:423:HIS:O	1:A:427:VAL:HG23	2.11	0.50
1:A:63:ARG:NH1	1:A:63:ARG:HB3	2.23	0.49
1:A:471:ASN:ND2	1:A:473:HIS:N	2.60	0.49
1:A:146:ALA:HB3	1:A:147:PRO:HD3	1.95	0.49
1:A:134:GLU:HG3	1:A:135:GLY:N	2.27	0.49
1:A:434:PRO:HG2	1:A:437:ASN:HB2	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASP:O	1:A:129:GLN:HB2	2.12	0.49
1:A:128:ARG:NH1	1:A:134:GLU:OE1	2.46	0.49
3:A:615:ANP:H5'1	4:A:655:HOH:O	2.12	0.49
1:A:354:GLN:HG3	1:A:416:MET:HE1	1.95	0.49
1:A:334:ARG:O	1:A:334:ARG:HG3	2.11	0.49
1:A:188:LEU:HD12	1:A:188:LEU:C	2.33	0.49
1:A:28:GLY:O	1:A:30:ALA:N	2.46	0.48
1:A:215:GLN:HG3	1:A:219:GLY:O	2.14	0.48
1:A:134:GLU:HG3	1:A:135:GLY:H	1.77	0.48
1:A:127:VAL:HB	1:A:138:LEU:HD11	1.95	0.48
1:A:602:SER:O	1:A:604:VAL:N	2.41	0.48
1:A:610:LEU:C	1:A:612:VAL:N	2.66	0.48
1:A:441:LEU:HD22	1:A:475:ALA:HB2	1.95	0.48
1:A:369:LYS:HZ2	1:A:479:ASP:CG	2.16	0.48
1:A:505:TRP:CZ2	1:A:539:PRO:HG2	2.49	0.48
1:A:332:LEU:HD21	1:A:403:GLY:HA3	1.96	0.48
1:A:572:MET:O	1:A:575:CYS:HB2	2.14	0.47
1:A:425:PHE:CD2	1:A:469:LEU:HD11	2.50	0.47
1:A:368:ILE:HD12	1:A:368:ILE:N	2.30	0.47
1:A:544:LYS:O	1:A:545:GLY:O	2.32	0.47
1:A:194:GLU:HB3	1:A:197:THR:OG1	2.15	0.47
1:A:544:LYS:HG3	1:A:545:GLY:H	1.79	0.47
1:A:133:LEU:HD23	1:A:138:LEU:HA	1.95	0.47
1:A:376:GLU:O	1:A:377:LYS:CB	2.63	0.47
1:A:544:LYS:NZ	4:A:657:HOH:O	2.48	0.47
1:A:440:GLU:OE2	1:A:473:HIS:HD2	1.98	0.47
1:A:239:LEU:HD13	1:A:246:LEU:HD11	1.97	0.47
1:A:460:ARG:HH11	1:A:460:ARG:HG3	1.79	0.47
1:A:146:ALA:N	1:A:147:PRO:CD	2.79	0.46
1:A:544:LYS:CG	1:A:545:GLY:N	2.77	0.46
1:A:188:LEU:C	1:A:189:LEU:HD12	2.36	0.46
1:A:604:VAL:CG2	1:A:605:GLU:N	2.69	0.46
1:A:108:LEU:HD12	1:A:109:GLU:H	1.81	0.46
1:A:577:ILE:O	1:A:583:ARG:HD3	2.16	0.46
1:A:64:GLN:HB2	1:A:66:ASN:OD1	2.16	0.46
1:A:223:ILE:HG22	1:A:235:LEU:HD21	1.97	0.45
1:A:525:TYR:OH	1:A:593:MET:HG3	2.15	0.45
1:A:460:ARG:HG2	1:A:516:PHE:HD2	1.81	0.45
1:A:568:LEU:HD22	1:A:593:MET:HE1	1.98	0.45
1:A:429:LYS:HD3	1:A:432:GLU:OE1	2.16	0.45
1:A:505:TRP:HZ2	1:A:531:GLU:CD	2.20	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:PHE:CD1	1:A:235:LEU:HG	2.52	0.44
1:A:568:LEU:HD22	1:A:593:MET:HE2	1.99	0.44
1:A:50:LEU:HD23	1:A:57:HIS:HB2	1.98	0.44
1:A:338:LEU:HD12	1:A:338:LEU:HA	1.85	0.44
1:A:462:LEU:HD23	1:A:525:TYR:N	2.33	0.44
1:A:203:ILE:HD11	1:A:208:VAL:HG22	1.98	0.44
1:A:164:TYR:HE2	1:A:166:SER:HG	1.63	0.44
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.75	0.44
1:A:480:PHE:O	1:A:480:PHE:CD1	2.71	0.44
1:A:41:ARG:HH12	1:A:226:GLY:C	2.21	0.44
1:A:337:LEU:CD2	1:A:339:ILE:HD11	2.48	0.44
1:A:440:GLU:HG3	1:A:597:TYR:OH	2.18	0.44
1:A:70:ALA:HB2	1:A:76:ALA:HA	1.99	0.43
1:A:175:ARG:HD3	1:A:175:ARG:O	2.18	0.43
1:A:607:GLY:O	1:A:608:SER:OG	2.26	0.43
1:A:119:ARG:HD3	4:A:662:HOH:O	2.18	0.43
1:A:450:LYS:HE3	1:A:587:LEU:CD1	2.47	0.43
1:A:231:THR:N	1:A:234:GLN:NE2	2.67	0.43
1:A:322:PRO:HG2	1:A:402:ILE:HD12	2.00	0.43
1:A:354:GLN:HG2	1:A:355:GLY:H	1.80	0.43
1:A:40:LEU:CD2	1:A:40:LEU:H	2.30	0.43
1:A:146:ALA:O	1:A:150:GLU:HG3	2.18	0.43
1:A:95:PRO:O	1:A:96:CYS:HB3	2.19	0.43
1:A:143:ILE:HB	1:A:447:MET:HE1	2.01	0.43
1:A:519:ARG:NH1	1:A:581:GLU:HA	2.34	0.43
1:A:523:TRP:O	1:A:527:VAL:HG23	2.19	0.43
1:A:399:VAL:HG21	1:A:478:SER:HB3	2.00	0.43
1:A:529:MET:CB	1:A:572:MET:HE2	2.48	0.43
1:A:519:ARG:HH12	1:A:581:GLU:HA	1.81	0.43
1:A:202:LEU:HD23	1:A:209:TYR:HB2	1.99	0.43
1:A:341:ASP:N	1:A:342:ILE:HD12	2.33	0.42
1:A:324:GLU:O	1:A:325:LEU:CB	2.67	0.42
1:A:41:ARG:HH22	1:A:226:GLY:CA	2.19	0.42
1:A:453:GLU:HG3	1:A:518:SER:CB	2.48	0.42
1:A:34:PHE:HA	1:A:49:SER:O	2.19	0.42
1:A:607:GLY:N	1:A:610:LEU:HD21	2.34	0.42
1:A:321:ASP:OD1	1:A:322:PRO:N	2.53	0.42
1:A:540:TYR:CE2	1:A:558:MET:HG3	2.55	0.42
1:A:177:LEU:HB3	1:A:203:ILE:HD11	2.01	0.42
1:A:551:PHE:CZ	1:A:556:LYS:HB3	2.55	0.42
1:A:612:VAL:HG12	1:A:612:VAL:O	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD22	1:A:40:LEU:N	2.31	0.42
1:A:370:VAL:O	1:A:371:LEU:O	2.38	0.42
1:A:445:VAL:O	1:A:449:MET:HG2	2.19	0.42
1:A:391:HIS:HE1	1:A:402:ILE:O	2.03	0.42
1:A:579:LYS:HB2	1:A:582:ASP:OD1	2.20	0.42
1:A:198:TYR:CE1	1:A:221:TYR:CE2	3.07	0.42
1:A:31:ASP:HA	1:A:51:VAL:O	2.20	0.42
1:A:314:VAL:HG12	1:A:314:VAL:O	2.19	0.41
1:A:202:LEU:HD21	1:A:209:TYR:HB2	2.01	0.41
1:A:437:ASN:HD22	1:A:472:ARG:HH21	1.69	0.41
1:A:533:LEU:HA	1:A:533:LEU:HD23	1.84	0.41
1:A:314:VAL:HG13	1:A:474:TYR:CD2	2.56	0.41
1:A:77:HIS:HE1	1:A:86:PHE:CG	2.38	0.41
1:A:561:PRO:HA	1:A:562:PRO:HD3	1.98	0.41
1:A:203:ILE:HD13	1:A:208:VAL:HG22	2.03	0.41
1:A:212:LEU:HD12	1:A:213:ILE:N	2.36	0.41
1:A:187:PHE:C	1:A:187:PHE:CD1	2.94	0.41
1:A:344:LEU:HD11	1:A:354:GLN:HB2	2.02	0.41
1:A:141:ALA:HB1	1:A:315:PHE:CE2	2.56	0.41
1:A:145:GLN:O	1:A:149:VAL:HG23	2.21	0.41
1:A:586:PHE:HA	1:A:589:VAL:HB	2.03	0.41
1:A:192:ARG:NH1	1:A:192:ARG:HB3	2.35	0.41
1:A:239:LEU:HB2	1:A:250:LEU:CD1	2.51	0.40
1:A:565:PRO:HB2	1:A:567:GLU:OE2	2.21	0.40
1:A:11:PHE:CZ	1:A:13:GLY:HA2	2.55	0.40
1:A:342:ILE:N	1:A:342:ILE:CD1	2.79	0.40
1:A:239:LEU:HA	1:A:242:LYS:O	2.21	0.40
1:A:449:MET:SD	1:A:477:ILE:HD13	2.61	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	539/613 (88%)	469 (87%)	53 (10%)	17 (3%)	5 8

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	MET
1	A	325	LEU
1	A	327	ASP
1	A	373	GLN
1	A	377	LYS
1	A	603	LYS
1	A	92	ASP
1	A	349	PHE
1	A	350	GLY
1	A	371	LEU
1	A	545	GLY
1	A	604	VAL
1	A	318	PRO
1	A	544	LYS
1	A	612	VAL
1	A	106	SER
1	A	580	TRP

### 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	430/519 (83%)	404 (94%)	26 (6%)	24 47

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	63	ARG
1	A	97	ASN
1	A	175	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	198	TYR
1	A	200	LEU
1	A	202	LEU
1	A	235	LEU
1	A	240	LYS
1	A	249	CYS
1	A	313	SER
1	A	315	PHE
1	A	318	PRO
1	A	320	SER
1	A	330	LEU
1	A	381	GLU
1	A	471	ASN
1	A	514	ARG
1	A	537	GLN
1	A	544	LYS
1	A	559	GLU
1	A	567	GLU
1	A	582	ASP
1	A	593	MET
1	A	605	GLU
1	A	610	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	97	ASN
1	A	129	GLN
1	A	140	GLN
1	A	234	GLN
1	A	256	ASN
1	A	336	ASN
1	A	354	GLN
1	A	391	HIS
1	A	395	ASN
1	A	437	ASN
1	A	471	ASN
1	A	473	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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	615	2	27,33,33	1.77	7 (25%)	30,52,52	1.75	7 (23%)

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	615	2	-	1/12/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	615	ANP	PB-O3A	-3.40	1.54	1.59
3	A	615	ANP	PB-O2B	-2.71	1.49	1.56
3	A	615	ANP	PG-O3G	-2.58	1.49	1.56
3	A	615	ANP	PG-O2G	-2.13	1.50	1.56

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	615	ANP	C4-N3	2.80	1.39	1.35
3	A	615	ANP	O4'-C1'	2.90	1.44	1.41
3	A	615	ANP	PG-O1G	4.46	1.51	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	615	ANP	O1G-PG-N3B	-4.29	105.32	111.90
3	A	615	ANP	C2'-C1'-N9	-2.41	110.61	114.29
3	A	615	ANP	O1B-PB-N3B	-2.38	108.24	111.90
3	A	615	ANP	O3A-PB-N3B	-2.17	100.47	106.44
3	A	615	ANP	PA-O3A-PB	2.47	140.93	132.67
3	A	615	ANP	C4'-O4'-C1'	2.86	112.86	109.72
3	A	615	ANP	O2B-PB-O1B	3.81	117.96	110.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	615	ANP	O1G-PG-N3B-PB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	615	ANP	1	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 [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, 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	545/613 (88%)	-0.03	4 (0%) 89 87	18, 42, 66, 79	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	613	ALA	2.7
1	A	2	PRO	2.6
1	A	349	PHE	2.4
1	A	483	SER	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<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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ANP	A	615	31/31	0.95	0.15	-0.58	27,37,48,52	0
2	MG	A	614	1/1	0.98	0.11	-	28,28,28,28	0

## 6.5 Other polymers

There are no such residues in this entry.