



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 08:26 AM BST

PDB ID : 1ANV  
Title : ADENOVIRUS 5 DBP/URANYL FLUORIDE SOAK  
Authors : Kanellopoulos, P.N.; Tsernoglou, D.; Van Der Vliet, P.C.; Tucker, P.A.  
Deposited on : 1996-03-14  
Resolution : 2.70 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

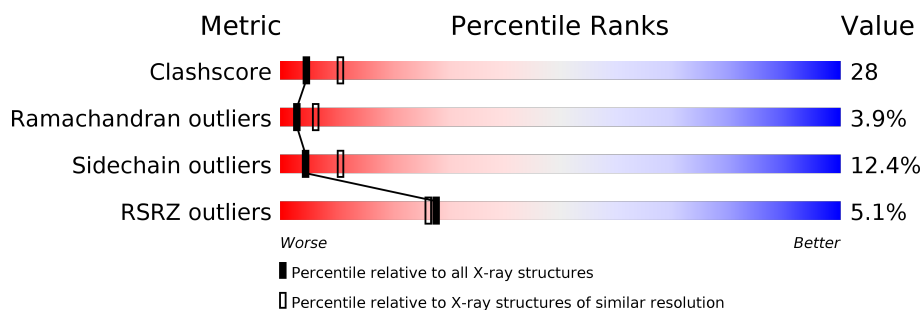
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	356	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2500 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.

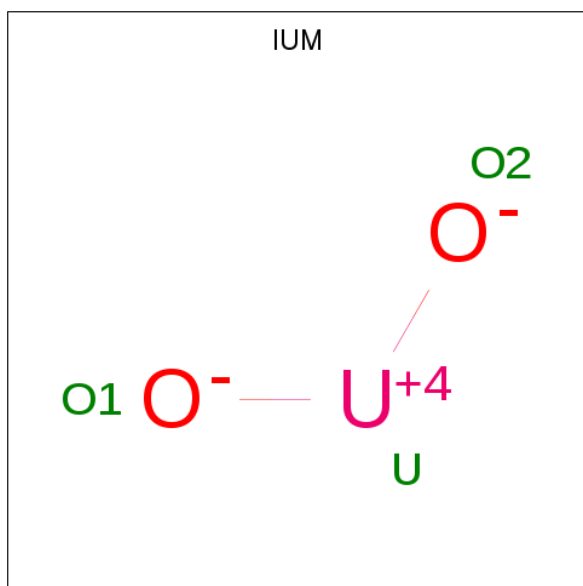
- Molecule 1 is a protein called ADENOVIRUS SINGLE-STRANDED DNA-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2463	1562	432	446	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is URANYL (VI) ION (three-letter code: IUM) (formula: O<sub>2</sub>U).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	U	0	0
			1	1		
3	A	1	Total	U	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	U	0	0
			1	1		
3	A	1	Total	U	0	0
			1	1		

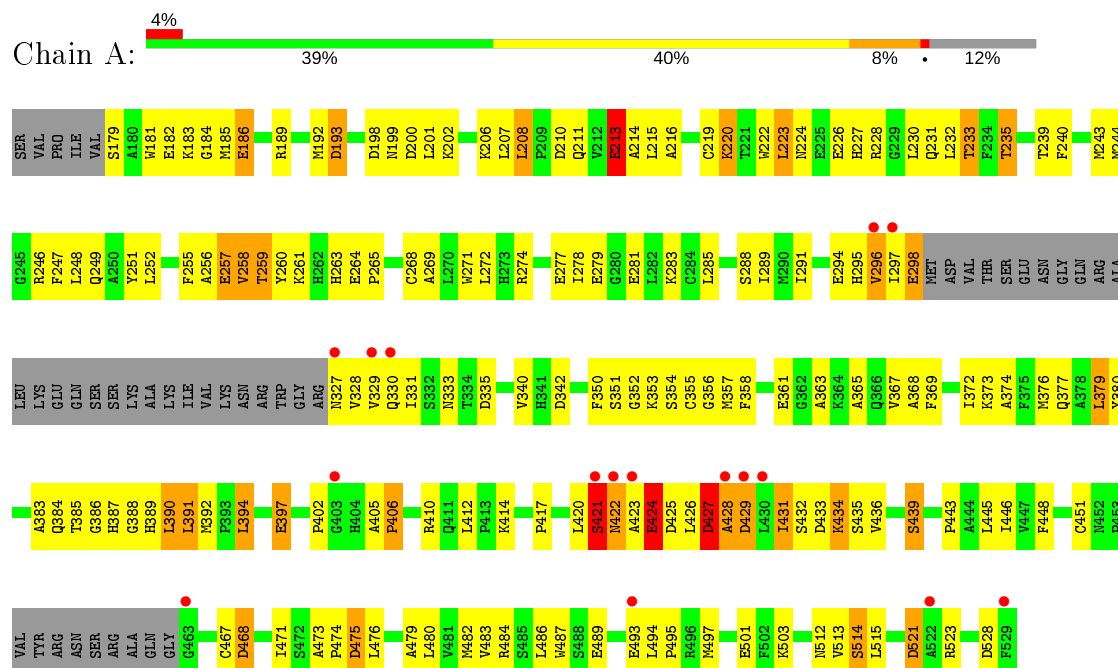
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		

### 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: ADENOVIRUS SINGLE-STRANDED DNA-BINDING PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.70Å 75.60Å 60.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 14.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.70) 93.8 (14.93-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.79 (at 2.69Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.204 , 0.310 0.194 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 99.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2500	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.73% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

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	0.77	13/2525 (0.5%)	1.09	23/3417 (0.7%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	493	GLU	CD-OE1	5.91	1.32	1.25
1	A	226	GLU	CD-OE2	5.79	1.32	1.25
1	A	361	GLU	CD-OE2	5.67	1.31	1.25
1	A	277	GLU	CD-OE1	5.61	1.31	1.25
1	A	294	GLU	CD-OE2	5.61	1.31	1.25
1	A	186	GLU	CD-OE1	5.54	1.31	1.25
1	A	489	GLU	CD-OE1	5.46	1.31	1.25
1	A	213	GLU	CD-OE2	5.44	1.31	1.25
1	A	264	GLU	CD-OE2	5.39	1.31	1.25
1	A	279	GLU	CD-OE2	5.35	1.31	1.25
1	A	182	GLU	CD-OE1	5.34	1.31	1.25
1	A	424	GLU	CD-OE2	5.30	1.31	1.25
1	A	397	GLU	CD-OE1	5.20	1.31	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	A	475	ASP	CB-CG-OD1	-7.82	111.27	118.30
1	A	475	ASP	CB-CG-OD2	7.36	124.92	118.30
1	A	193	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	521	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	A	198	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	A	198	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	468	ASP	CB-CG-OD1	6.25	123.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	433	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	A	468	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	A	246	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	200	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	200	ASP	CB-CG-OD1	-5.86	113.02	118.30
1	A	335	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	429	ASP	CB-CG-OD1	-5.85	113.03	118.30
1	A	521	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	528	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	210	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	433	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	427	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	425	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	528	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2463	0	2400	137	1
2	A	2	0	0	0	0
3	A	4	0	0	0	1
4	A	31	0	0	5	0
All	All	2500	0	2400	137	1

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 (137) 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:269:ALA:HB2	1:A:394:LEU:HD21	1.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:THR:HB	1:A:471:ILE:HA	1.39	1.01
1:A:263:HIS:CE1	1:A:402:PRO:HG2	2.07	0.89
1:A:379:LEU:HB3	1:A:380:TYR:CD1	2.16	0.81
1:A:269:ALA:CB	1:A:394:LEU:HD21	2.12	0.78
1:A:222:TRP:CD1	1:A:486:LEU:HD13	2.23	0.74
1:A:181:TRP:HZ2	1:A:206:LYS:HD2	1.53	0.73
1:A:272:LEU:HD23	1:A:274:ARG:CZ	2.19	0.72
1:A:374:ALA:HA	1:A:377:GLN:HE21	1.54	0.71
1:A:295:HIS:HB2	1:A:333:ASN:HB2	1.74	0.70
1:A:230:LEU:HD12	1:A:231:GLN:H	1.57	0.70
1:A:199:ASN:HD22	1:A:202:LYS:HE3	1.56	0.69
1:A:373:LYS:O	1:A:377:GLN:HG3	1.92	0.69
1:A:514:SER:O	1:A:515:LEU:HD23	1.93	0.69
1:A:424:GLU:OE2	1:A:443:PRO:HB3	1.94	0.68
1:A:263:HIS:HE1	1:A:402:PRO:HG2	1.57	0.67
1:A:479:ALA:O	1:A:483:VAL:HG23	1.95	0.66
1:A:342:ASP:OD1	1:A:354:SER:HB2	1.96	0.65
1:A:291:ILE:N	1:A:291:ILE:HD13	2.13	0.64
1:A:473:ALA:HB3	1:A:474:PRO:HD3	1.79	0.63
1:A:421:SER:O	1:A:423:ALA:N	2.30	0.63
1:A:255:PHE:HB2	1:A:495:PRO:HG3	1.81	0.62
1:A:431:ILE:HG21	1:A:436:VAL:HG11	1.81	0.62
1:A:184:GLY:HA3	1:A:207:LEU:HD11	1.81	0.62
1:A:363:ALA:O	1:A:367:VAL:HG23	1.99	0.62
1:A:446:ILE:N	4:A:23:HOH:O	2.32	0.61
1:A:391:LEU:HD13	1:A:476:LEU:HG	1.83	0.61
1:A:278:ILE:HB	1:A:281:GLU:HB3	1.81	0.61
1:A:355:CYS:SG	1:A:357:MET:HB3	2.42	0.60
1:A:420:LEU:O	1:A:421:SER:C	2.39	0.60
1:A:247:PHE:HB2	1:A:483:VAL:HG21	1.84	0.60
1:A:353:LYS:NZ	4:A:2:HOH:O	2.32	0.60
1:A:181:TRP:CZ2	1:A:206:LYS:HD2	2.35	0.59
1:A:327:ASN:O	1:A:328:VAL:HG13	2.03	0.58
1:A:421:SER:O	1:A:422:ASN:C	2.41	0.58
1:A:421:SER:O	1:A:424:GLU:N	2.38	0.57
1:A:206:LYS:HB2	1:A:208:LEU:HD22	1.87	0.57
1:A:397:GLU:HB3	1:A:467:CYS:SG	2.44	0.57
1:A:424:GLU:HG2	1:A:424:GLU:O	2.04	0.57
1:A:487:TRP:CD1	1:A:494:LEU:HD12	2.39	0.57
1:A:434:LYS:HZ2	1:A:434:LYS:HB2	1.70	0.56
1:A:372:ILE:O	1:A:376:MET:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:GLU:HB3	1:A:467:CYS:CB	2.36	0.56
1:A:331:ILE:N	1:A:331:ILE:HD12	2.21	0.55
1:A:379:LEU:HD22	1:A:380:TYR:HE1	1.72	0.55
1:A:394:LEU:HA	1:A:412:LEU:HD22	1.88	0.55
1:A:223:LEU:O	1:A:227:HIS:N	2.40	0.55
1:A:379:LEU:HB3	1:A:380:TYR:CE1	2.41	0.55
1:A:199:ASN:HD22	1:A:202:LYS:CE	2.20	0.55
1:A:445:LEU:HA	4:A:23:HOH:O	2.06	0.55
1:A:230:LEU:HD12	1:A:231:GLN:N	2.22	0.54
1:A:365:ALA:O	1:A:369:PHE:HD2	1.90	0.54
1:A:514:SER:C	1:A:515:LEU:HD23	2.28	0.54
1:A:386:GLY:O	1:A:388:GLY:N	2.35	0.54
1:A:392:MET:CE	1:A:394:LEU:HD11	2.38	0.53
1:A:183:LYS:HD3	1:A:256:ALA:HA	1.89	0.53
1:A:185:MET:O	1:A:189:ARG:HB2	2.09	0.53
1:A:476:LEU:O	1:A:476:LEU:HD12	2.10	0.52
1:A:235:THR:HG21	1:A:475:ASP:CB	2.39	0.52
1:A:230:LEU:HD21	1:A:482:MET:CE	2.39	0.52
1:A:410:ARG:HG2	1:A:412:LEU:O	2.10	0.51
1:A:272:LEU:O	1:A:274:ARG:HD2	2.11	0.50
1:A:232:LEU:HB3	1:A:235:THR:HG23	1.94	0.50
1:A:379:LEU:HD22	1:A:380:TYR:CE1	2.46	0.50
1:A:368:ALA:HB1	1:A:446:ILE:HG13	1.94	0.50
1:A:208:LEU:HB2	1:A:211:GLN:OE1	2.11	0.49
1:A:268:CYS:HB3	1:A:392:MET:O	2.12	0.49
1:A:420:LEU:O	1:A:422:ASN:OD1	2.30	0.49
1:A:421:SER:H	1:A:443:PRO:HB2	1.78	0.49
1:A:369:PHE:O	1:A:372:ILE:HG22	2.12	0.49
1:A:383:ALA:O	1:A:385:THR:N	2.45	0.49
1:A:260:TYR:HB2	1:A:263:HIS:HB2	1.95	0.48
1:A:480:LEU:O	1:A:484:ARG:HG3	2.12	0.48
1:A:421:SER:OG	1:A:422:ASN:N	2.45	0.48
1:A:417:PRO:HA	1:A:445:LEU:O	2.13	0.48
1:A:256:ALA:O	1:A:257:GLU:HB2	2.14	0.48
1:A:298:GLU:OE2	1:A:330:GLN:OE1	2.30	0.48
1:A:271:TRP:CE2	1:A:285:LEU:HD23	2.49	0.48
1:A:263:HIS:ND1	1:A:402:PRO:HG2	2.27	0.47
1:A:431:ILE:HG21	1:A:436:VAL:CG1	2.43	0.47
1:A:296:VAL:C	1:A:297:ILE:HG12	2.35	0.47
1:A:272:LEU:HG	1:A:272:LEU:O	2.15	0.47
1:A:431:ILE:HG22	1:A:432:SER:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:GLY:CA	1:A:512:ASN:ND2	2.78	0.47
1:A:350:PHE:N	1:A:350:PHE:CD1	2.83	0.47
1:A:434:LYS:NZ	1:A:434:LYS:HB2	2.30	0.46
1:A:219:CYS:O	1:A:223:LEU:HB2	2.15	0.46
1:A:239:THR:O	1:A:243:MET:HG2	2.16	0.46
1:A:480:LEU:O	1:A:480:LEU:HD12	2.16	0.46
1:A:222:TRP:O	1:A:223:LEU:C	2.54	0.45
1:A:340:VAL:HG12	4:A:1:HOH:O	2.16	0.45
1:A:206:LYS:O	1:A:211:GLN:OE1	2.34	0.45
1:A:281:GLU:OE2	1:A:283:LYS:HE3	2.16	0.45
1:A:405:ALA:O	1:A:406:PRO:C	2.55	0.45
1:A:295:HIS:CE1	1:A:358:PHE:CZ	3.05	0.45
1:A:352:GLY:N	1:A:512:ASN:ND2	2.65	0.45
1:A:230:LEU:HD21	1:A:482:MET:HE1	1.98	0.44
1:A:352:GLY:HA2	1:A:512:ASN:HD22	1.82	0.44
1:A:427:ASP:O	1:A:428:ALA:HB2	2.17	0.44
1:A:251:TYR:CE1	1:A:497:MET:HB2	2.53	0.44
1:A:296:VAL:HG13	1:A:330:GLN:HG3	1.99	0.44
1:A:189:ARG:HA	1:A:192:MET:HE2	2.00	0.44
1:A:261:LYS:HA	4:A:20:HOH:O	2.17	0.44
1:A:269:ALA:HB2	1:A:394:LEU:CD2	2.28	0.44
1:A:392:MET:HE3	1:A:394:LEU:CD1	2.47	0.44
1:A:208:LEU:HD12	1:A:208:LEU:HA	1.73	0.43
1:A:410:ARG:HG2	1:A:412:LEU:H	1.82	0.43
1:A:258:VAL:HG23	1:A:259:THR:N	2.33	0.43
1:A:414:LYS:O	1:A:448:PHE:HA	2.18	0.43
1:A:521:ASP:C	1:A:523:ARG:H	2.21	0.43
1:A:220:LYS:HE3	1:A:220:LYS:HB2	1.56	0.43
1:A:379:LEU:HB3	1:A:380:TYR:HD1	1.78	0.43
1:A:513:VAL:HG22	1:A:515:LEU:HD21	2.00	0.43
1:A:329:VAL:O	1:A:331:ILE:HD12	2.19	0.42
1:A:420:LEU:CD2	1:A:439:SER:HB3	2.49	0.42
1:A:352:GLY:HA2	1:A:512:ASN:ND2	2.35	0.42
1:A:215:LEU:HD12	1:A:249:GLN:HB2	2.02	0.42
1:A:230:LEU:HD21	1:A:482:MET:HE3	2.02	0.41
1:A:240:PHE:O	1:A:244:MET:HG3	2.20	0.41
1:A:420:LEU:HD23	1:A:424:GLU:OE1	2.18	0.41
1:A:223:LEU:HD12	1:A:227:HIS:HB2	2.02	0.41
1:A:350:PHE:CD2	1:A:356:GLY:HA2	2.55	0.41
1:A:383:ALA:C	1:A:385:THR:H	2.23	0.41
1:A:295:HIS:CE1	1:A:358:PHE:HZ	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASN:OD1	1:A:423:ALA:N	2.44	0.41
1:A:271:TRP:O	1:A:389:HIS:HA	2.21	0.41
1:A:426:LEU:O	1:A:427:ASP:HB3	2.20	0.41
1:A:392:MET:HE2	1:A:394:LEU:HD11	2.03	0.41
1:A:412:LEU:O	1:A:451:CYS:HA	2.21	0.41
1:A:271:TRP:HE3	1:A:390:LEU:HD23	1.85	0.41
1:A:230:LEU:CD2	1:A:482:MET:HE3	2.51	0.40
1:A:410:ARG:O	1:A:451:CYS:HB3	2.22	0.40
1:A:213:GLU:CD	1:A:214:ALA:H	2.25	0.40
1:A:213:GLU:O	1:A:216:ALA:N	2.55	0.40
1:A:392:MET:CE	1:A:394:LEU:CD1	3.00	0.40
1:A:230:LEU:CD2	1:A:482:MET:CE	2.99	0.40
1:A:222:TRP:CG	1:A:486:LEU:HD13	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASP:OD1	3:A:532:IUM:U[2_665]	2.12	0.08

## 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	308/356 (86%)	262 (85%)	34 (11%)	12 (4%)	<b>3</b> <b>6</b>

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	ASN
1	A	428	ALA
1	A	431	ILE

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Mol	Chain	Res	Type
1	A	233	THR
1	A	384	GLN
1	A	427	ASP
1	A	429	ASP
1	A	224	ASN
1	A	387	HIS
1	A	421	SER
1	A	296	VAL
1	A	265	PRO

### 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	267/303 (88%)	234 (88%)	33 (12%)	4 11

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	SER
1	A	186	GLU
1	A	201	LEU
1	A	208	LEU
1	A	213	GLU
1	A	220	LYS
1	A	223	LEU
1	A	228	ARG
1	A	233	THR
1	A	235	THR
1	A	248	LEU
1	A	252	LEU
1	A	257	GLU
1	A	258	VAL
1	A	259	THR
1	A	288	SER
1	A	289	ILE

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Mol	Chain	Res	Type
1	A	298	GLU
1	A	351	SER
1	A	379	LEU
1	A	390	LEU
1	A	391	LEU
1	A	394	LEU
1	A	406	PRO
1	A	421	SER
1	A	424	GLU
1	A	434	LYS
1	A	435	SER
1	A	439	SER
1	A	468	ASP
1	A	501	GLU
1	A	503	LYS
1	A	514	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	A	295	HIS
1	A	327	ASN
1	A	333	ASN
1	A	377	GLN
1	A	382	ASN
1	A	512	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic and 4 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	314/356 (88%)	-0.25	16 (5%) 28 26	6, 26, 70, 99	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	ILE	6.7
1	A	428	ALA	6.0
1	A	421	SER	5.5
1	A	429	ASP	3.5
1	A	422	ASN	3.5
1	A	296	VAL	3.4
1	A	430	LEU	3.1
1	A	463	GLY	3.1
1	A	329	VAL	2.9
1	A	522	ALA	2.6
1	A	493	GLU	2.6
1	A	529	PHE	2.4
1	A	330	GLN	2.3
1	A	423	ALA	2.3
1	A	327	ASN	2.3
1	A	403	GLY	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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	IUM	A	535	1/3	0.96	0.03	57,57,57,57	0
3	IUM	A	534	1/3	0.98	0.04	61,61,61,61	0
3	IUM	A	532	1/3	0.99	0.04	42,42,42,42	0
3	IUM	A	533	1/3	0.99	0.04	56,56,56,56	0
2	ZN	A	531	1/1	0.99	0.03	25,25,25,25	0
2	ZN	A	530	1/1	1.00	0.06	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.