



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:56 PM GMT

PDB ID : 1D9Z  
Title : CRYSTAL STRUCTURE OF THE DNA REPAIR PROTEIN UVRB IN COMPLEX WITH ATP  
Authors : Theis, K.; Chen, P.J.; Skovvaga, M.; Van Houten, B.; Kisker, C.  
Deposited on : 1999-10-30  
Resolution : 3.15 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

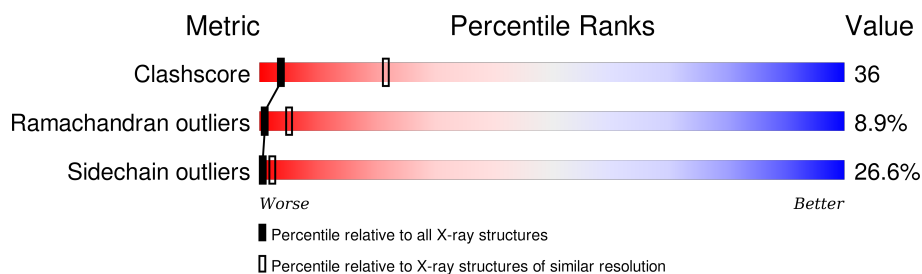
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	657	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4666 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 EXCINUCLEASE UVRABC COMPONENT UVRB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	0	0
			4632	2916	826	879	11			

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

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



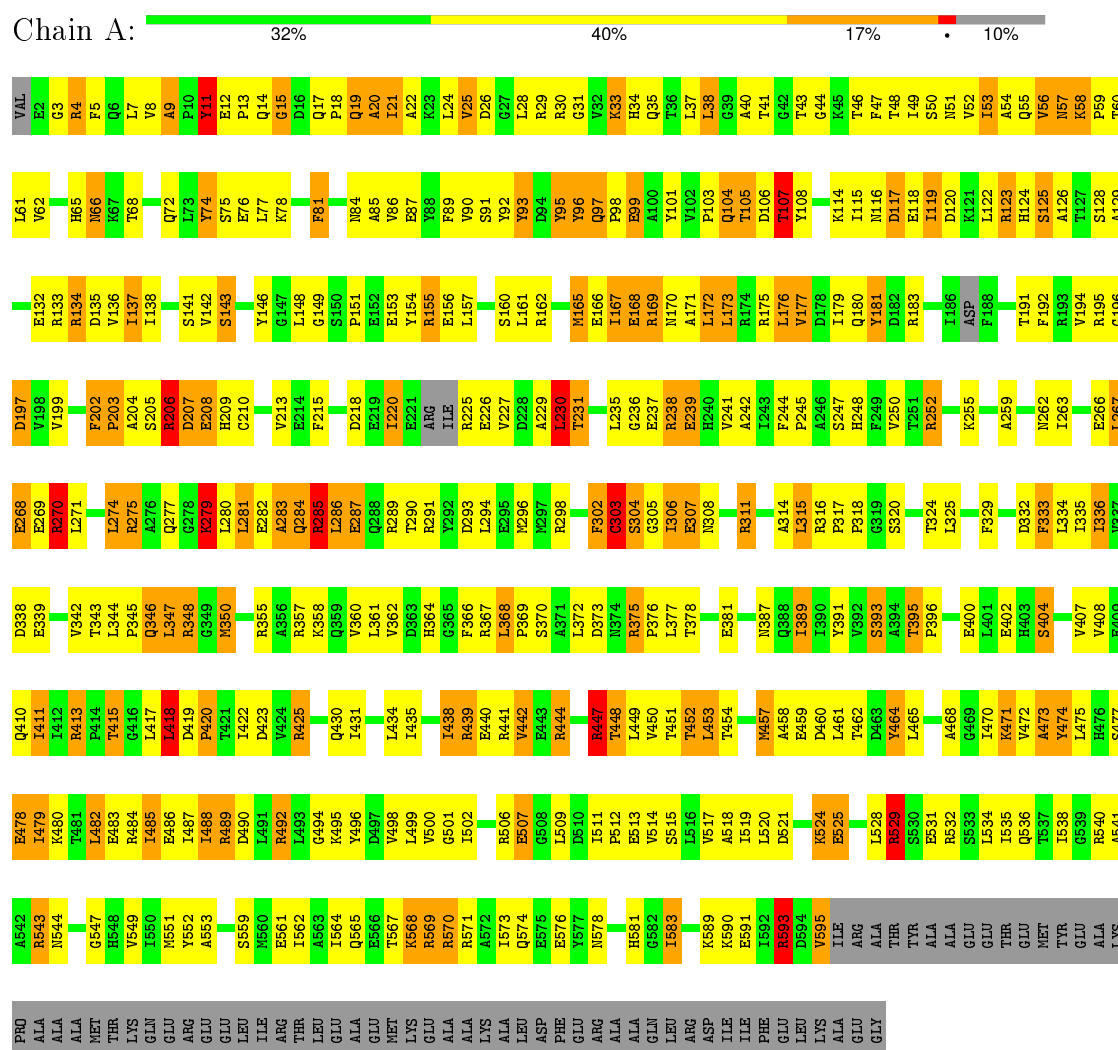
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: EXCINUCLEASE UVRABC COMPONENT UVRB



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.44Å 153.44Å 80.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.15	Depositor
% Data completeness (in resolution range)	100.0 (20.00-3.15)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC, XPLOR	Depositor
R, $R_{free}$	0.262 , 0.335	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4666	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.48	0/4705	1.22	33/6365 (0.5%)

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

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	ARG	NE-CZ-NH2	-15.08	112.76	120.30
1	A	441	ARG	NE-CZ-NH2	-14.12	113.24	120.30
1	A	570	ARG	NE-CZ-NH1	13.09	126.84	120.30
1	A	348	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	A	348	ARG	NE-CZ-NH2	-10.69	114.96	120.30
1	A	311	ARG	NH1-CZ-NH2	8.93	129.23	119.40
1	A	441	ARG	NH1-CZ-NH2	7.96	128.15	119.40
1	A	270	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	A	413	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	529	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	A	206	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	A	203	PRO	N-CA-CB	6.71	111.35	103.30
1	A	506	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	A	492	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	285	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	A	423	ASP	CB-CG-OD2	6.53	124.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ARG	CD-NE-CZ	6.34	132.47	123.60
1	A	474	TYR	CG-CD1-CE1	6.29	126.33	121.30
1	A	570	ARG	NH1-CZ-NH2	-6.17	112.61	119.40
1	A	206	ARG	NH1-CZ-NH2	-5.62	113.22	119.40
1	A	569	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	A	529	ARG	NH1-CZ-NH2	5.45	125.39	119.40
1	A	129	ALA	N-CA-CB	-5.45	102.48	110.10
1	A	474	TYR	CB-CG-CD1	5.42	124.25	121.00
1	A	553	ALA	N-CA-CB	-5.30	102.69	110.10
1	A	206	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	A	238	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	543	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	439	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	447	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	A	418	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	444	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	367	ARG	CA-CB-CG	5.10	124.61	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	THR	Mainchain
1	A	268	GLU	Mainchain
1	A	279	LYS	Mainchain

## 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	4632	0	4574	330	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	31	0	12	2	0
All	All	4666	0	4586	330	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 36.

All (330) 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:168:GLU:HG3	1:A:170:ASN:H	1.26	1.01
1:A:60:THR:HG21	1:A:334:LEU:HD23	1.50	0.92
1:A:90:VAL:HG22	1:A:91:SER:H	1.41	0.85
1:A:168:GLU:HB3	1:A:171:ALA:HB2	1.57	0.84
1:A:447:ARG:HB2	1:A:514:VAL:HG23	1.63	0.81
1:A:449:LEU:HD22	1:A:499:LEU:HD22	1.64	0.80
1:A:521:ASP:H	1:A:529:ARG:HH21	1.27	0.79
1:A:58:LYS:HG3	1:A:134:ARG:HH12	1.46	0.79
1:A:475:LEU:O	1:A:475:LEU:HD22	1.84	0.78
1:A:473:ALA:HB3	1:A:499:LEU:HA	1.65	0.76
1:A:471:LYS:HB3	1:A:496:TYR:HA	1.69	0.74
1:A:454:THR:OG1	1:A:457:MET:HB2	1.88	0.73
1:A:168:GLU:HB3	1:A:171:ALA:CB	2.18	0.73
1:A:279:LYS:HA	1:A:282:GLU:HA	1.70	0.73
1:A:274:LEU:HB3	1:A:283:ALA:HB1	1.71	0.72
1:A:490:ASP:O	1:A:495:LYS:HB2	1.90	0.72
1:A:24:LEU:HA	1:A:35:GLN:HE22	1.54	0.72
1:A:101:TYR:O	1:A:103:PRO:HD3	1.90	0.72
1:A:281:LEU:HB2	1:A:285:ARG:HH12	1.54	0.72
1:A:40:ALA:O	1:A:43:THR:HG23	1.90	0.71
1:A:271:LEU:O	1:A:275:ARG:HB2	1.91	0.71
1:A:450:VAL:HG13	1:A:518:ALA:HB3	1.72	0.71
1:A:60:THR:HG22	1:A:334:LEU:HB3	1.72	0.71
1:A:434:LEU:O	1:A:434:LEU:HG	1.90	0.71
1:A:570:ARG:O	1:A:574:GLN:HG3	1.91	0.71
1:A:226:GLU:H	1:A:226:GLU:CD	1.94	0.70
1:A:247:SER:HB3	1:A:250:VAL:HG23	1.72	0.70
1:A:451:THR:HG22	1:A:519:ILE:HA	1.74	0.70
1:A:474:TYR:HD1	1:A:475:LEU:N	1.90	0.69
1:A:473:ALA:CB	1:A:499:LEU:HA	2.21	0.69
1:A:58:LYS:HG3	1:A:134:ARG:NH1	2.07	0.69
1:A:368:LEU:HB2	1:A:369:PRO:HD2	1.75	0.69
1:A:286:LEU:HD23	1:A:287:GLU:N	2.08	0.68
1:A:155:ARG:O	1:A:155:ARG:HD3	1.92	0.68
1:A:400:GLU:O	1:A:404:SER:HB2	1.93	0.68
1:A:375:ARG:HB2	1:A:376:PRO:HD2	1.76	0.68
1:A:28:LEU:HD13	1:A:56:VAL:HG11	1.76	0.67
1:A:230:LEU:HD23	1:A:231:THR:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:HD23	1:A:500:VAL:HG21	1.76	0.66
1:A:85:ALA:HB1	1:A:136:VAL:HG13	1.77	0.66
1:A:46:THR:O	1:A:49:ILE:HG22	1.95	0.66
1:A:85:ALA:HB3	1:A:136:VAL:HA	1.78	0.65
1:A:274:LEU:HD22	1:A:283:ALA:HA	1.77	0.65
1:A:498:VAL:HG12	1:A:499:LEU:H	1.62	0.65
1:A:101:TYR:HD1	1:A:108:TYR:HA	1.62	0.64
1:A:368:LEU:HD23	1:A:368:LEU:H	1.62	0.64
1:A:531:GLU:HG3	1:A:562:ILE:HG21	1.79	0.64
1:A:284:GLN:O	1:A:285:ARG:HB3	1.97	0.64
1:A:86:VAL:HG22	1:A:137:ILE:CG2	2.28	0.63
1:A:358:LYS:O	1:A:362:VAL:HG23	1.99	0.63
1:A:498:VAL:HG12	1:A:499:LEU:N	2.14	0.63
1:A:459:GLU:OE1	1:A:475:LEU:HD11	1.99	0.63
1:A:452:THR:HG21	1:A:457:MET:HB3	1.80	0.63
1:A:104:GLN:H	1:A:104:GLN:NE2	1.96	0.62
1:A:149:GLY:HA3	1:A:248:HIS:O	2.00	0.62
1:A:60:THR:HG22	1:A:334:LEU:CB	2.30	0.61
1:A:578:ASN:HA	1:A:583:ILE:HD12	1.82	0.61
1:A:565:GLN:HA	1:A:565:GLN:OE1	2.00	0.61
1:A:435:ILE:O	1:A:438:ILE:HG22	2.00	0.61
1:A:581:HIS:HB2	1:A:583:ILE:HD11	1.83	0.61
1:A:285:ARG:HG3	1:A:286:LEU:N	2.15	0.60
1:A:170:ASN:OD1	1:A:173:LEU:HD22	2.01	0.60
1:A:521:ASP:HB3	1:A:524:LYS:HG2	1.82	0.60
1:A:474:TYR:CD1	1:A:475:LEU:N	2.68	0.60
1:A:419:ASP:O	1:A:571:ARG:HD2	2.00	0.60
1:A:90:VAL:HG22	1:A:91:SER:N	2.13	0.60
1:A:17:GLN:HB2	1:A:18:PRO:HD3	1.83	0.60
1:A:284:GLN:O	1:A:285:ARG:CB	2.49	0.59
1:A:286:LEU:HD23	1:A:287:GLU:H	1.66	0.59
1:A:470:ILE:O	1:A:472:VAL:HG23	2.03	0.59
1:A:225:ARG:O	1:A:227:VAL:HG22	2.03	0.58
1:A:25:VAL:O	1:A:26:ASP:C	2.41	0.58
1:A:368:LEU:N	1:A:368:LEU:HD23	2.18	0.58
1:A:458:ALA:HB3	1:A:475:LEU:HD23	1.85	0.58
1:A:229:ALA:O	1:A:230:LEU:HB2	2.02	0.58
1:A:325:LEU:HD12	1:A:325:LEU:O	2.03	0.58
1:A:59:PRO:HD3	1:A:134:ARG:HH11	1.68	0.58
1:A:488:ILE:HD11	1:A:509:LEU:HD23	1.85	0.58
1:A:280:LEU:HD12	1:A:280:LEU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HA	1:A:125:SER:OG	2.03	0.57
1:A:172:LEU:O	1:A:176:LEU:HB2	2.05	0.57
1:A:284:GLN:HG3	1:A:285:ARG:N	2.19	0.57
1:A:92:TYR:HE1	1:A:115:ILE:HD13	1.69	0.57
1:A:268:GLU:O	1:A:270:ARG:N	2.37	0.57
1:A:172:LEU:HD12	1:A:172:LEU:O	2.05	0.57
1:A:281:LEU:HG	1:A:285:ARG:HB3	1.86	0.57
1:A:431:ILE:O	1:A:435:ILE:HG13	2.04	0.57
1:A:459:GLU:HA	1:A:475:LEU:HG	1.87	0.57
1:A:281:LEU:HB2	1:A:285:ARG:NH1	2.19	0.57
1:A:393:SER:O	1:A:396:PRO:HD3	2.05	0.57
1:A:173:LEU:O	1:A:177:VAL:HG22	2.06	0.56
1:A:98:PRO:O	1:A:99:GLU:C	2.44	0.56
1:A:311:ARG:HG3	1:A:373:ASP:HB3	1.87	0.56
1:A:377:LEU:HD22	1:A:381:GLU:HB3	1.87	0.56
1:A:333:PHE:H	1:A:333:PHE:HD2	1.52	0.56
1:A:512:PRO:HD2	1:A:513:GLU:OE2	2.06	0.55
1:A:116:ASN:O	1:A:118:GLU:N	2.39	0.55
1:A:485:ILE:HG23	1:A:595:VAL:HG11	1.88	0.55
1:A:528:LEU:O	1:A:529:ARG:HD3	2.06	0.55
1:A:38:LEU:HD12	1:A:38:LEU:C	2.27	0.55
1:A:85:ALA:CB	1:A:136:VAL:HG13	2.36	0.55
1:A:105:THR:O	1:A:106:ASP:C	2.44	0.55
1:A:4:ARG:HG3	1:A:4:ARG:HH11	1.72	0.54
1:A:306:ILE:HG23	1:A:307:GLU:N	2.22	0.54
1:A:395:THR:HB	1:A:532:ARG:HG2	1.89	0.54
1:A:448:THR:O	1:A:449:LEU:HD23	2.07	0.54
1:A:13:PRO:HA	1:A:17:GLN:OE1	2.07	0.54
1:A:151:PRO:O	1:A:154:TYR:HB3	2.08	0.54
1:A:44:GLY:HA3	4:A:700:ATP:H8	1.72	0.54
1:A:314:ALA:O	1:A:315:LEU:HB2	2.08	0.54
1:A:447:ARG:HB2	1:A:514:VAL:CG2	2.35	0.54
1:A:29:ARG:O	1:A:31:GLY:N	2.41	0.54
1:A:105:THR:HB	1:A:107:THR:OG1	2.08	0.54
1:A:408:VAL:HG12	1:A:408:VAL:O	2.07	0.54
1:A:578:ASN:HA	1:A:583:ILE:CD1	2.38	0.54
1:A:199:VAL:HA	1:A:220:ILE:CB	2.38	0.54
1:A:502:ILE:N	1:A:502:ILE:HD12	2.23	0.54
1:A:482:LEU:O	1:A:485:ILE:HG22	2.07	0.53
1:A:483:GLU:HG2	1:A:487:ILE:HD11	1.89	0.53
1:A:472:VAL:HG12	1:A:473:ALA:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD23	1:A:268:GLU:N	2.24	0.53
1:A:50:SER:HB3	1:A:81:PHE:CZ	2.44	0.53
1:A:93:TYR:CD2	1:A:143:SER:HB3	2.43	0.53
1:A:461:LEU:HD23	1:A:500:VAL:CG2	2.39	0.53
1:A:239:GLU:CD	1:A:239:GLU:N	2.62	0.53
1:A:21:ILE:HD13	1:A:51:ASN:CB	2.39	0.53
1:A:86:VAL:HG22	1:A:137:ILE:HG22	1.91	0.53
1:A:531:GLU:O	1:A:535:ILE:HD12	2.09	0.53
1:A:20:ALA:O	1:A:21:ILE:C	2.47	0.52
1:A:291:ARG:HH11	1:A:291:ARG:HG3	1.72	0.52
1:A:487:ILE:HA	1:A:490:ASP:HB2	1.90	0.52
1:A:266:GLU:CD	1:A:368:LEU:HD12	2.30	0.52
1:A:551:MET:CE	1:A:564:ILE:HD11	2.40	0.52
1:A:28:LEU:O	1:A:31:GLY:N	2.39	0.52
1:A:531:GLU:HG3	1:A:562:ILE:CG2	2.39	0.52
1:A:75:SER:OG	1:A:76:GLU:N	2.43	0.52
1:A:302:PHE:O	1:A:303:CYS:HB3	2.10	0.52
1:A:24:LEU:HA	1:A:35:GLN:NE2	2.22	0.52
1:A:5:PHE:HD2	1:A:84:ASN:OD1	1.93	0.52
1:A:53:ILE:HG22	1:A:54:ALA:N	2.24	0.52
1:A:168:GLU:HG3	1:A:170:ASN:N	2.10	0.51
1:A:459:GLU:HG3	1:A:475:LEU:HG	1.92	0.51
1:A:458:ALA:CB	1:A:475:LEU:HD23	2.40	0.51
1:A:479:ILE:H	1:A:479:ILE:HD12	1.75	0.51
1:A:168:GLU:HG3	1:A:169:ARG:N	2.26	0.51
1:A:418:LEU:N	1:A:418:LEU:HD12	2.26	0.50
1:A:59:PRO:HD3	1:A:134:ARG:NH1	2.26	0.50
1:A:490:ASP:HB3	1:A:496:TYR:CE1	2.46	0.50
1:A:338:ASP:OD2	1:A:339:GLU:HG2	2.10	0.50
1:A:517:VAL:HB	1:A:549:VAL:HG22	1.94	0.50
1:A:335:ILE:HB	1:A:389:ILE:HG23	1.92	0.50
1:A:509:LEU:HA	1:A:511:ILE:HD11	1.94	0.50
1:A:62:VAL:HG13	1:A:336:ILE:HG22	1.94	0.50
1:A:116:ASN:O	1:A:119:ILE:HG12	2.11	0.50
1:A:420:PRO:HG3	1:A:541:ALA:O	2.12	0.50
1:A:270:ARG:HD3	1:A:270:ARG:O	2.12	0.49
1:A:285:ARG:HH11	1:A:285:ARG:CB	2.25	0.49
1:A:60:THR:HG21	1:A:334:LEU:CD2	2.32	0.49
1:A:535:ILE:O	1:A:538:ILE:HB	2.12	0.49
1:A:439:ARG:O	1:A:442:VAL:HG12	2.12	0.49
1:A:458:ALA:HB3	1:A:475:LEU:CD2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:GLN:HG3	1:A:431:ILE:HD13	1.94	0.49
1:A:33:LYS:HB3	1:A:34:HIS:CD2	2.48	0.49
1:A:17:GLN:O	1:A:21:ILE:HG13	2.13	0.49
1:A:77:LEU:HD23	1:A:81:PHE:HE1	1.78	0.49
1:A:4:ARG:NH1	1:A:4:ARG:HG3	2.27	0.49
1:A:344:LEU:HD11	1:A:391:TYR:CE2	2.48	0.48
1:A:21:ILE:HG12	1:A:48:THR:HG23	1.94	0.48
1:A:101:TYR:CD1	1:A:108:TYR:HA	2.46	0.48
1:A:478:GLU:HG3	1:A:478:GLU:H	1.48	0.48
1:A:368:LEU:CB	1:A:369:PRO:HD2	2.38	0.48
1:A:512:PRO:HA	1:A:543:ARG:HB3	1.94	0.48
1:A:92:TYR:HB3	1:A:96:TYR:HD1	1.78	0.48
1:A:375:ARG:HB2	1:A:376:PRO:CD	2.43	0.48
1:A:593:ARG:HG2	1:A:593:ARG:H	1.38	0.48
1:A:97:GLN:HA	1:A:98:PRO:HD3	1.73	0.47
1:A:270:ARG:O	1:A:274:LEU:HB2	2.13	0.47
1:A:512:PRO:O	1:A:544:ASN:ND2	2.45	0.47
1:A:173:LEU:O	1:A:173:LEU:HG	2.15	0.47
1:A:332:ASP:HA	1:A:387:ASN:ND2	2.30	0.47
1:A:490:ASP:OD2	1:A:495:LYS:HE3	2.14	0.47
1:A:87:GLU:OE1	1:A:125:SER:HB2	2.14	0.47
1:A:335:ILE:O	1:A:389:ILE:HG22	2.15	0.47
1:A:138:ILE:HD12	1:A:329:PHE:CZ	2.49	0.47
1:A:56:VAL:O	1:A:57:ASN:C	2.53	0.47
1:A:289:ARG:O	1:A:293:ASP:HB2	2.14	0.47
1:A:8:VAL:O	1:A:9:ALA:HB2	2.14	0.47
1:A:60:THR:CG2	1:A:334:LEU:HD23	2.34	0.46
1:A:448:THR:HG22	1:A:449:LEU:H	1.81	0.46
1:A:21:ILE:HD13	1:A:51:ASN:HB2	1.97	0.46
1:A:60:THR:HB	1:A:334:LEU:O	2.16	0.46
1:A:146:TYR:O	1:A:324:THR:HG22	2.15	0.46
1:A:267:LEU:O	1:A:267:LEU:HG	2.14	0.46
1:A:37:LEU:HD11	1:A:410:GLN:HE21	1.78	0.46
1:A:44:GLY:HA3	4:A:700:ATP:C8	2.51	0.46
1:A:335:ILE:HB	1:A:389:ILE:CG2	2.45	0.46
1:A:161:LEU:HB2	1:A:241:VAL:HG12	1.98	0.46
1:A:347:LEU:HA	1:A:350:MET:HG3	1.97	0.46
1:A:123:ARG:NH1	1:A:123:ARG:HG2	2.31	0.46
1:A:89:PHE:CD1	1:A:325:LEU:HD22	2.51	0.46
1:A:284:GLN:CG	1:A:285:ARG:N	2.74	0.45
1:A:502:ILE:H	1:A:502:ILE:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:O	1:A:369:PRO:C	2.53	0.45
1:A:499:LEU:O	1:A:499:LEU:HD23	2.16	0.45
1:A:29:ARG:C	1:A:31:GLY:H	2.20	0.45
1:A:168:GLU:CG	1:A:170:ASN:H	2.13	0.45
1:A:86:VAL:HA	1:A:137:ILE:O	2.17	0.45
1:A:179:ILE:O	1:A:180:GLN:C	2.52	0.45
1:A:14:GLN:O	1:A:15:GLY:C	2.55	0.45
1:A:447:ARG:HH12	1:A:494:GLY:N	2.14	0.45
1:A:531:GLU:CG	1:A:562:ILE:HG21	2.47	0.45
1:A:65:HIS:O	1:A:66:ASN:HB3	2.17	0.45
1:A:207:ASP:O	1:A:209:HIS:N	2.35	0.45
1:A:85:ALA:O	1:A:137:ILE:N	2.44	0.45
1:A:317:PRO:HA	1:A:318:PRO:HD3	1.80	0.45
1:A:157:LEU:HD11	1:A:252:ARG:HE	1.82	0.45
1:A:205:SER:O	1:A:206:ARG:C	2.55	0.45
1:A:103:PRO:HB3	1:A:364:HIS:CE1	2.51	0.45
1:A:551:MET:HE2	1:A:564:ILE:HD11	1.99	0.45
1:A:7:LEU:HD12	1:A:8:VAL:O	2.17	0.45
1:A:461:LEU:O	1:A:462:THR:C	2.55	0.44
1:A:34:HIS:N	1:A:34:HIS:CD2	2.85	0.44
1:A:411:ILE:H	1:A:411:ILE:HD13	1.82	0.44
1:A:20:ALA:O	1:A:21:ILE:O	2.35	0.44
1:A:488:ILE:CG2	1:A:489:ARG:N	2.80	0.44
1:A:267:LEU:O	1:A:271:LEU:HD23	2.17	0.44
1:A:281:LEU:HD23	1:A:285:ARG:NH1	2.32	0.44
1:A:47:PHE:O	1:A:48:THR:C	2.55	0.44
1:A:306:ILE:CG2	1:A:307:GLU:N	2.80	0.44
1:A:49:ILE:CG2	1:A:50:SER:N	2.80	0.44
1:A:241:VAL:HG22	1:A:242:ALA:H	1.82	0.44
1:A:345:PRO:O	1:A:348:ARG:HB3	2.18	0.44
1:A:196:GLY:O	1:A:197:ASP:CB	2.66	0.44
1:A:472:VAL:HG12	1:A:473:ALA:H	1.83	0.44
1:A:87:GLU:HG3	1:A:126:ALA:HA	2.00	0.44
1:A:333:PHE:N	1:A:387:ASN:HD22	2.15	0.44
1:A:492:ARG:HH22	1:A:590:LYS:CB	2.31	0.44
1:A:285:ARG:HB3	1:A:285:ARG:HH11	1.82	0.44
1:A:368:LEU:HB2	1:A:369:PRO:CD	2.44	0.44
1:A:108:TYR:HE1	1:A:366:PHE:HD1	1.66	0.44
1:A:226:GLU:HG2	1:A:238:ARG:O	2.18	0.44
1:A:581:HIS:HB2	1:A:583:ILE:CD1	2.48	0.44
1:A:11:TYR:HB2	1:A:12:GLU:H	1.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PRO:HB3	1:A:547:GLY:O	2.18	0.43
1:A:490:ASP:HB3	1:A:496:TYR:HE1	1.82	0.43
1:A:230:LEU:HD23	1:A:231:THR:N	2.30	0.43
1:A:461:LEU:O	1:A:464:TYR:N	2.51	0.43
1:A:50:SER:HB3	1:A:81:PHE:HZ	1.82	0.43
1:A:375:ARG:CB	1:A:376:PRO:HD2	2.46	0.43
1:A:62:VAL:HG22	1:A:336:ILE:HB	1.99	0.43
1:A:279:LYS:CA	1:A:282:GLU:HA	2.43	0.43
1:A:120:ASP:OD2	1:A:124:HIS:CE1	2.72	0.43
1:A:176:LEU:O	1:A:181:TYR:HA	2.18	0.43
1:A:471:LYS:HG2	1:A:495:LYS:O	2.19	0.43
1:A:156:GLU:HG2	1:A:252:ARG:NH2	2.33	0.43
1:A:500:VAL:HG12	1:A:501:GLY:N	2.34	0.43
1:A:534:LEU:O	1:A:535:ILE:C	2.57	0.43
1:A:183:ARG:CB	1:A:206:ARG:HB3	2.48	0.43
1:A:434:LEU:O	1:A:438:ILE:HB	2.19	0.43
1:A:5:PHE:HD1	1:A:57:ASN:HA	1.84	0.43
1:A:123:ARG:HH11	1:A:123:ARG:HG2	1.82	0.43
1:A:165:MET:HG3	1:A:165:MET:H	1.65	0.43
1:A:306:ILE:HG23	1:A:307:GLU:H	1.84	0.43
1:A:364:HIS:HB3	1:A:366:PHE:CE2	2.54	0.43
1:A:74:TYR:HE1	1:A:86:VAL:HG12	1.84	0.43
1:A:306:ILE:CG2	1:A:307:GLU:H	2.32	0.43
1:A:180:GLN:CB	1:A:302:PHE:HE2	2.32	0.43
1:A:81:PHE:CD1	1:A:81:PHE:N	2.86	0.42
1:A:92:TYR:HE2	1:A:119:ILE:HG13	1.83	0.42
1:A:453:LEU:HD23	1:A:453:LEU:HA	1.84	0.42
1:A:103:PRO:HB3	1:A:364:HIS:HE1	1.85	0.42
1:A:524:LYS:HD2	1:A:524:LYS:HA	1.75	0.42
1:A:372:LEU:O	1:A:375:ARG:HG2	2.18	0.42
1:A:167:ILE:HG22	1:A:171:ALA:HB3	2.01	0.42
1:A:279:LYS:H	1:A:280:LEU:HD12	1.85	0.42
1:A:415:THR:OG1	1:A:417:LEU:HD12	2.18	0.42
1:A:142:VAL:HG11	1:A:346:GLN:OE1	2.20	0.42
1:A:569:ARG:O	1:A:573:ILE:HG13	2.19	0.42
1:A:274:LEU:HD22	1:A:283:ALA:CA	2.47	0.42
1:A:255:LYS:HG2	1:A:315:LEU:CD2	2.48	0.42
1:A:74:TYR:O	1:A:78:LYS:HG3	2.19	0.42
1:A:378:THR:HG1	1:A:381:GLU:CD	2.23	0.42
1:A:305:GLY:O	1:A:306:ILE:C	2.57	0.42
1:A:192:PHE:O	1:A:202:PHE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PRO:O	1:A:19:GLN:C	2.58	0.42
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.87	0.42
1:A:66:ASN:OD1	1:A:66:ASN:C	2.57	0.42
1:A:40:ALA:HB3	1:A:43:THR:CG2	2.49	0.42
1:A:52:VAL:O	1:A:56:VAL:HG22	2.20	0.42
1:A:333:PHE:N	1:A:333:PHE:CD2	2.88	0.42
1:A:425:ARG:O	1:A:552:TYR:HA	2.19	0.42
1:A:450:VAL:HG12	1:A:451:THR:H	1.85	0.42
1:A:153:GLU:OE2	1:A:255:LYS:HE3	2.20	0.42
1:A:65:HIS:O	1:A:65:HIS:ND1	2.53	0.42
1:A:498:VAL:CG1	1:A:499:LEU:H	2.30	0.41
1:A:135:ASP:OD2	1:A:135:ASP:O	2.37	0.41
1:A:104:GLN:C	1:A:106:ASP:H	2.23	0.41
1:A:342:VAL:O	1:A:345:PRO:HG2	2.20	0.41
1:A:452:THR:HG22	1:A:453:LEU:H	1.85	0.41
1:A:21:ILE:HG22	1:A:22:ALA:N	2.35	0.41
1:A:119:ILE:HB	1:A:120:ASP:H	1.69	0.41
1:A:75:SER:O	1:A:76:GLU:C	2.58	0.41
1:A:259:ALA:O	1:A:262:ASN:HB2	2.19	0.41
1:A:360:VAL:CG1	1:A:361:LEU:N	2.83	0.41
1:A:485:ILE:HG23	1:A:595:VAL:CG1	2.49	0.41
1:A:551:MET:HE1	1:A:564:ILE:HD11	2.01	0.41
1:A:511:ILE:HA	1:A:512:PRO:HD3	1.80	0.41
1:A:303:CYS:SG	1:A:304:SER:N	2.94	0.41
1:A:498:VAL:CG1	1:A:499:LEU:N	2.81	0.41
1:A:85:ALA:HB3	1:A:135:ASP:O	2.19	0.41
1:A:447:ARG:NH1	1:A:494:GLY:N	2.69	0.41
1:A:86:VAL:HG22	1:A:137:ILE:HG21	2.03	0.41
1:A:525:GLU:H	1:A:525:GLU:HG2	1.67	0.41
1:A:519:ILE:HG22	1:A:519:ILE:O	2.21	0.41
1:A:578:ASN:OD1	1:A:583:ILE:HB	2.21	0.41
1:A:418:LEU:N	1:A:418:LEU:CD1	2.84	0.41
1:A:274:LEU:CD2	1:A:283:ALA:HA	2.48	0.40
1:A:239:GLU:CD	1:A:239:GLU:H	2.25	0.40
1:A:338:ASP:O	1:A:339:GLU:C	2.60	0.40
1:A:60:THR:CG2	1:A:334:LEU:HB3	2.43	0.40
1:A:74:TYR:CE1	1:A:86:VAL:HG12	2.56	0.40
1:A:218:ASP:HA	1:A:225:ARG:C	2.41	0.40
1:A:517:VAL:CG2	1:A:541:ALA:HB2	2.52	0.40
1:A:177:VAL:HA	1:A:181:TYR:HB3	2.04	0.40
1:A:450:VAL:HG12	1:A:451:THR:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:CD2	1:A:231:THR:H	2.32	0.40
1:A:407:VAL:HG23	1:A:408:VAL:N	2.36	0.40
1:A:465:LEU:O	1:A:468:ALA:HB3	2.21	0.40
1:A:306:ILE:O	1:A:308:ASN:N	2.54	0.40
1:A:244:PHE:HA	1:A:245:PRO:HD3	1.90	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	584/657 (89%)	435 (74%)	97 (17%)	52 (9%)	<b>1</b> <b>5</b>

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	95	TYR
1	A	96	TYR
1	A	99	GLU
1	A	117	ASP
1	A	181	TYR
1	A	206	ARG
1	A	210	CYS
1	A	215	PHE
1	A	284	GLN
1	A	304	SER
1	A	507	GLU
1	A	15	GLY
1	A	74	TYR
1	A	119	ILE
1	A	197	ASP

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Mol	Chain	Res	Type
1	A	208	GLU
1	A	269	GLU
1	A	283	ALA
1	A	285	ARG
1	A	306	ILE
1	A	320	SER
1	A	477	SER
1	A	593	ARG
1	A	11	TYR
1	A	25	VAL
1	A	30	ARG
1	A	143	SER
1	A	168	GLU
1	A	191	THR
1	A	230	LEU
1	A	279	LYS
1	A	303	CYS
1	A	307	GLU
1	A	202	PHE
1	A	204	ALA
1	A	236	GLY
1	A	343	THR
1	A	370	SER
1	A	480	LYS
1	A	568	LYS
1	A	9	ALA
1	A	57	ASN
1	A	194	VAL
1	A	195	ARG
1	A	203	PRO
1	A	220	ILE
1	A	20	ALA
1	A	473	ALA
1	A	3	GLY
1	A	213	VAL
1	A	420	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	482/569 (85%)	354 (73%)	128 (27%)	0 2

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	11	TYR
1	A	19	GLN
1	A	33	LYS
1	A	38	LEU
1	A	41	THR
1	A	53	ILE
1	A	55	GLN
1	A	56	VAL
1	A	58	LYS
1	A	61	LEU
1	A	66	ASN
1	A	68	THR
1	A	72	GLN
1	A	81	PHE
1	A	93	TYR
1	A	95	TYR
1	A	97	GLN
1	A	104	GLN
1	A	105	THR
1	A	107	THR
1	A	114	LYS
1	A	117	ASP
1	A	123	ARG
1	A	125	SER
1	A	128	SER
1	A	132	GLU
1	A	133	ARG
1	A	134	ARG
1	A	137	ILE
1	A	141	SER
1	A	148	LEU
1	A	155	ARG
1	A	160	SER
1	A	162	ARG

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Mol	Chain	Res	Type
1	A	165	MET
1	A	166	GLU
1	A	167	ILE
1	A	169	ARG
1	A	172	LEU
1	A	173	LEU
1	A	175	ARG
1	A	176	LEU
1	A	177	VAL
1	A	207	ASP
1	A	208	GLU
1	A	230	LEU
1	A	231	THR
1	A	235	LEU
1	A	237	GLU
1	A	239	GLU
1	A	252	ARG
1	A	263	ILE
1	A	267	LEU
1	A	270	ARG
1	A	274	LEU
1	A	275	ARG
1	A	277	GLN
1	A	281	LEU
1	A	285	ARG
1	A	286	LEU
1	A	287	GLU
1	A	290	THR
1	A	294	LEU
1	A	296	MET
1	A	298	ARG
1	A	302	PHE
1	A	303	CYS
1	A	315	LEU
1	A	316	ARG
1	A	333	PHE
1	A	336	ILE
1	A	346	GLN
1	A	347	LEU
1	A	350	MET
1	A	355	ARG
1	A	357	ARG

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Mol	Chain	Res	Type
1	A	368	LEU
1	A	375	ARG
1	A	389	ILE
1	A	393	SER
1	A	395	THR
1	A	402	GLU
1	A	404	SER
1	A	411	ILE
1	A	413	ARG
1	A	415	THR
1	A	418	LEU
1	A	422	ILE
1	A	425	ARG
1	A	438	ILE
1	A	440	GLU
1	A	442	VAL
1	A	444	ARG
1	A	447	ARG
1	A	448	THR
1	A	452	THR
1	A	453	LEU
1	A	457	MET
1	A	460	ASP
1	A	464	TYR
1	A	471	LYS
1	A	478	GLU
1	A	479	ILE
1	A	482	LEU
1	A	484	ARG
1	A	485	ILE
1	A	486	GLU
1	A	488	ILE
1	A	489	ARG
1	A	507	GLU
1	A	515	SER
1	A	520	LEU
1	A	524	LYS
1	A	525	GLU
1	A	529	ARG
1	A	536	GLN
1	A	540	ARG
1	A	559	SER

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	561	GLU
1	A	567	THR
1	A	568	LYS
1	A	576	GLU
1	A	583	ILE
1	A	589	LYS
1	A	591	GLU
1	A	593	ARG
1	A	595	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	34	HIS
1	A	35	GLN
1	A	104	GLN
1	A	240	HIS
1	A	374	ASN
1	A	384	GLN
1	A	387	ASN
1	A	410	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are 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$
4	ATP	A	700	2	24,33,33	1.30	4 (16%)	31,52,52	2.71	9 (29%)

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
4	ATP	A	700	2	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	ATP	C8-N7	-3.25	1.28	1.34
4	A	700	ATP	C5-N7	-2.24	1.31	1.39
4	A	700	ATP	PB-O2B	-2.01	1.46	1.54
4	A	700	ATP	C2-N1	2.75	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	ATP	PA-O3A-PB	-7.88	110.59	132.73
4	A	700	ATP	O3A-PA-O5'	-4.92	89.89	102.94
4	A	700	ATP	PB-O3B-PG	-4.00	119.25	132.67
4	A	700	ATP	O2B-PB-O3B	2.11	114.64	105.09
4	A	700	ATP	O5'-PA-O1A	2.31	118.58	109.62
4	A	700	ATP	C4-C5-N7	3.34	112.55	109.48
4	A	700	ATP	C4'-O4'-C1'	3.84	113.93	109.72
4	A	700	ATP	C1'-N9-C4	5.64	135.45	126.94
4	A	700	ATP	O4'-C1'-N9	6.13	120.93	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	ATP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.