



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 10:20 AM EDT

PDB ID : 1R7R
Title : The crystal structure of murine p97/VCP at 3.6Å
Authors : Huyton, T.; Pye, V.E.; Briggs, L.C.; Flynn, T.C.; Beuron, F.; Kondo, H.; Ma, J.; Zhang, X.; Freemont, P.S.
Deposited on : unknown
Resolution : 3.60 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

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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

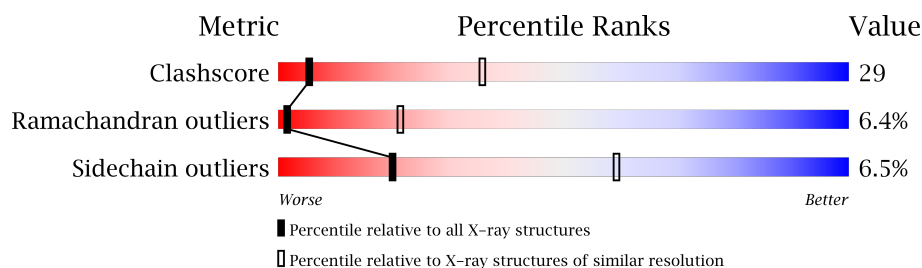
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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))
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	816	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4680 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.

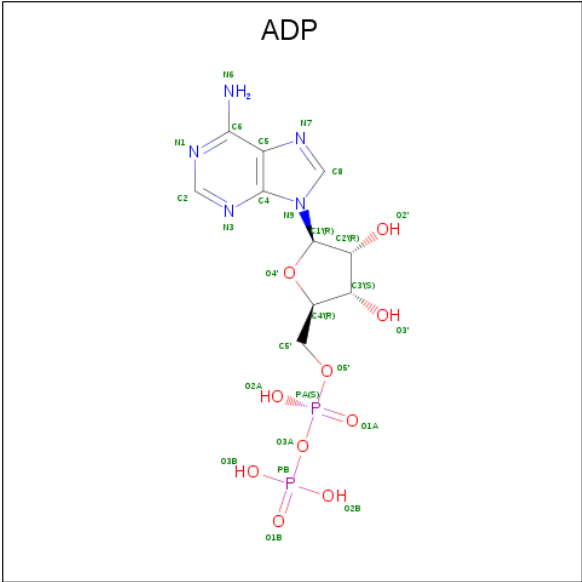
- Molecule 1 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	683	4653	2882	854	899	18	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	807	ALA	-	EXPRESSION TAG	UNP Q01853
A	808	ALA	-	EXPRESSION TAG	UNP Q01853
A	809	LEU	-	EXPRESSION TAG	UNP Q01853
A	810	GLU	-	EXPRESSION TAG	UNP Q01853
A	811	HIS	-	EXPRESSION TAG	UNP Q01853
A	812	HIS	-	EXPRESSION TAG	UNP Q01853
A	813	HIS	-	EXPRESSION TAG	UNP Q01853
A	814	HIS	-	EXPRESSION TAG	UNP Q01853
A	815	HIS	-	EXPRESSION TAG	UNP Q01853
A	816	HIS	-	EXPRESSION TAG	UNP Q01853

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



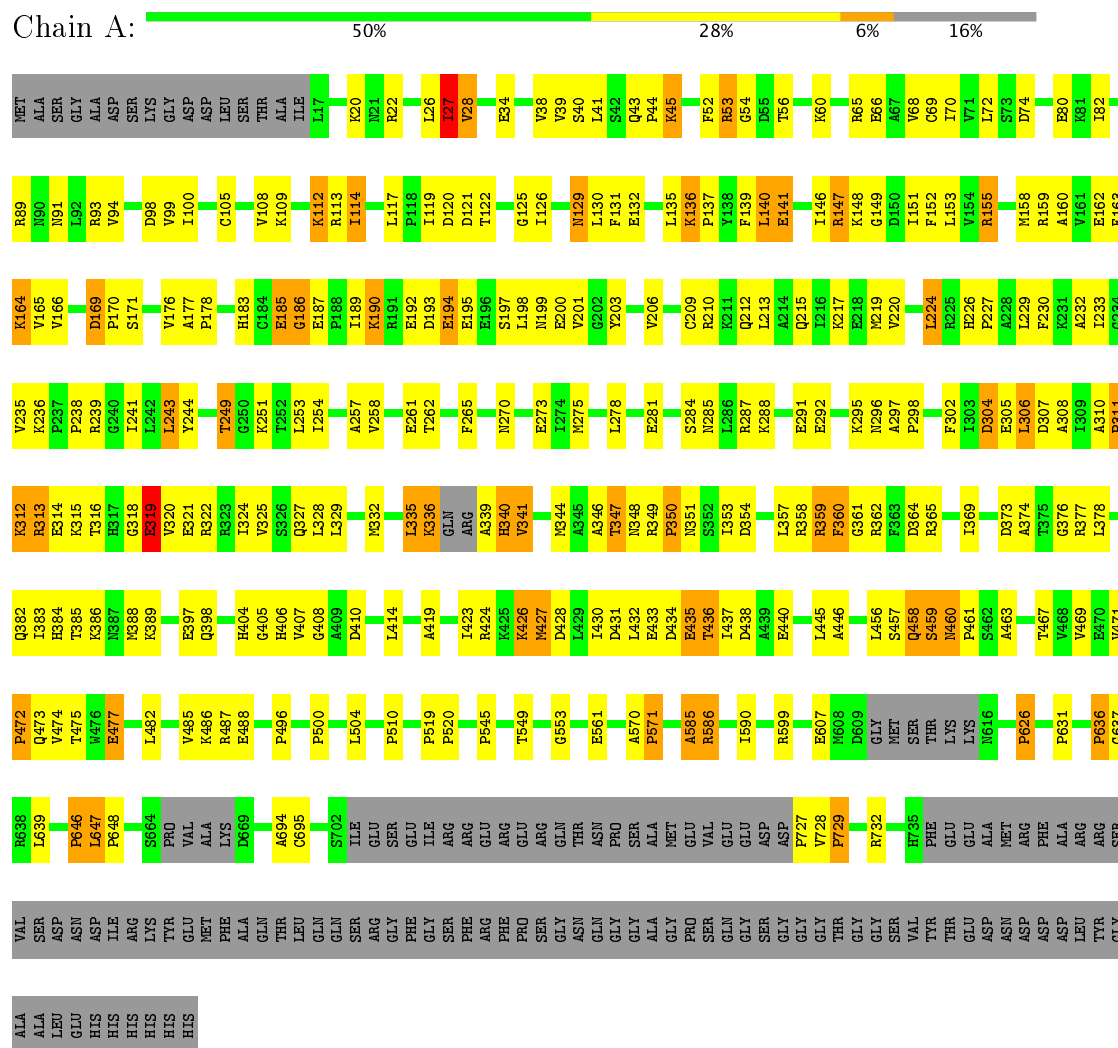
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

- Molecule 1: Transitional endoplasmic reticulum ATPase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	145.20 Å 145.20 Å 167.40 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 3.60	Depositor
% Data completeness (in resolution range)	98.5 (19.99-3.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.327 , 0.358	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4680	wwPDB-VP
Average B, all atoms (Å ²)	104.0	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: ADP

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	3/4703 (0.1%)	0.81	29/6394 (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	3	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	477	GLU	C-N	-16.57	0.95	1.34
1	A	27	ILE	C-N	-6.26	1.19	1.34
1	A	488	GLU	C-N	5.48	1.46	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	GLU	O-C-N	-17.77	94.27	122.70
1	A	27	ILE	O-C-N	-13.03	101.85	122.70
1	A	477	GLU	C-N-CA	11.11	149.48	121.70
1	A	477	GLU	CA-C-N	8.68	136.30	117.20
1	A	485	VAL	CA-C-N	-7.92	99.78	117.20
1	A	27	ILE	CA-C-N	7.79	134.33	117.20
1	A	186	GLY	N-CA-C	6.99	130.57	113.10
1	A	553	GLY	N-CA-C	6.44	129.20	113.10
1	A	647	LEU	N-CA-C	6.40	128.28	111.00
1	A	607	GLU	N-CA-C	6.01	127.23	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	GLN	N-CA-C	5.99	127.17	111.00
1	A	519	PRO	N-CA-CB	5.96	110.45	103.30
1	A	631	PRO	N-CA-CB	5.93	110.41	103.30
1	A	520	PRO	N-CA-CB	5.91	110.39	103.30
1	A	729	PRO	N-CA-CB	5.88	110.36	103.30
1	A	545	PRO	N-CA-CB	5.87	110.34	103.30
1	A	727	PRO	N-CA-CB	5.87	110.34	103.30
1	A	500	PRO	N-CA-CB	5.82	110.29	103.30
1	A	496	PRO	N-CA-CB	5.82	110.28	103.30
1	A	510	PRO	N-CA-CB	5.78	110.23	103.30
1	A	648	PRO	N-CA-CB	5.66	110.09	103.30
1	A	571	PRO	N-CA-CB	5.53	109.94	103.30
1	A	646	PRO	N-CA-CB	5.49	109.89	103.30
1	A	636	PRO	N-CA-CB	5.46	109.85	103.30
1	A	472	PRO	N-CA-CB	5.37	109.75	103.30
1	A	626	PRO	N-CA-CB	5.32	109.69	103.30
1	A	486	LYS	C-N-CA	5.23	134.78	121.70
1	A	485	VAL	O-C-N	5.12	130.89	122.70
1	A	457	SER	N-CA-CB	5.06	118.09	110.50

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	458	GLN	CA
1	A	607	GLU	CA
1	A	647	LEU	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	ILE	Mainchain
1	A	477	GLU	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	4653	0	4081	253	8
2	A	27	0	12	3	0
All	All	4680	0	4093	253	8

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 29.

All (253) 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:695:CYS:O	1:A:728:VAL:CB	1.94	1.15
1:A:312:LYS:HA	1:A:316:THR:HB	1.34	1.10
1:A:373:ASP:HB2	1:A:469:VAL:CB	1.83	1.09
1:A:427:MET:O	1:A:430:ILE:HG12	1.58	1.03
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.42	1.01
1:A:694:ALA:HB3	1:A:732:ARG:CB	1.99	0.91
1:A:694:ALA:CB	1:A:732:ARG:CB	2.49	0.90
1:A:129:ASN:ND2	1:A:132:GLU:H	1.69	0.90
1:A:353:ILE:HG23	1:A:357:LEU:HD12	1.56	0.88
1:A:27:ILE:HD13	1:A:99:VAL:HG12	1.57	0.87
1:A:203:TYR:CE2	1:A:261:GLU:HG2	2.10	0.86
1:A:373:ASP:HB2	1:A:469:VAL:CA	2.04	0.86
1:A:190:LYS:H	1:A:190:LYS:HD3	1.40	0.86
1:A:373:ASP:CB	1:A:469:VAL:CB	2.54	0.84
1:A:26:LEU:HD21	1:A:45:LYS:HE2	1.60	0.83
1:A:91:ASN:HD21	1:A:151:ILE:H	1.28	0.82
1:A:194:GLU:H	1:A:194:GLU:CD	1.81	0.82
1:A:312:LYS:HG3	1:A:316:THR:HG21	1.63	0.81
1:A:312:LYS:HA	1:A:316:THR:CB	2.12	0.80
1:A:129:ASN:HD21	1:A:132:GLU:H	1.31	0.79
1:A:129:ASN:C	1:A:129:ASN:HD22	1.84	0.78
1:A:177:ALA:HB1	1:A:178:PRO:HD2	1.65	0.78
1:A:239:ARG:HD3	1:A:336:LYS:HD2	1.64	0.78
1:A:254:ILE:CD1	1:A:369:ILE:HD13	2.15	0.76
1:A:169:ASP:HB3	1:A:170:PRO:CD	2.16	0.76
1:A:254:ILE:HD12	1:A:369:ILE:CD1	2.17	0.75
1:A:254:ILE:HD12	1:A:369:ILE:HD13	1.68	0.74
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.68	0.74
1:A:424:ARG:O	1:A:428:ASP:HB3	1.87	0.74
1:A:460:ASN:H	1:A:461:PRO:CD	2.03	0.72
1:A:206:VAL:HG22	1:A:253:LEU:HD22	1.71	0.72
1:A:435:GLU:HG3	1:A:436:THR:HG22	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:TYR:CE2	1:A:217:LYS:HE2	2.25	0.72
1:A:460:ASN:H	1:A:461:PRO:HD2	1.55	0.71
1:A:350:PRO:HB3	1:A:358:ARG:HH22	1.56	0.71
1:A:292:GLU:HG3	1:A:295:LYS:NZ	2.07	0.70
1:A:147:ARG:HD3	1:A:148:LYS:O	1.92	0.70
1:A:249:THR:HG23	1:A:369:ILE:CG2	2.21	0.69
1:A:426:LYS:HE2	1:A:426:LYS:HA	1.74	0.69
1:A:694:ALA:HB1	1:A:732:ARG:CB	2.21	0.69
1:A:347:THR:HG23	1:A:349:ARG:H	1.55	0.69
1:A:119:ILE:HD11	1:A:151:ILE:HD13	1.73	0.69
1:A:373:ASP:CG	1:A:469:VAL:CB	2.61	0.69
1:A:220:VAL:HB	1:A:224:LEU:HD22	1.75	0.68
1:A:215:GLN:O	1:A:219:MET:HG3	1.93	0.68
1:A:120:ASP:OD2	1:A:190:LYS:HA	1.96	0.66
1:A:318:GLY:O	1:A:322:ARG:HG2	1.96	0.66
1:A:254:ILE:CD1	1:A:369:ILE:CD1	2.74	0.65
1:A:335:LEU:O	1:A:336:LYS:HB2	1.96	0.65
1:A:117:LEU:HD13	1:A:187:GLU:O	1.95	0.65
1:A:378:LEU:HD23	1:A:397:GLU:HA	1.79	0.65
1:A:373:ASP:HB2	1:A:469:VAL:HA	1.78	0.64
1:A:445:LEU:HD23	1:A:446:ALA:N	2.13	0.64
1:A:336:LYS:HA	1:A:340:HIS:CE1	2.33	0.64
1:A:249:THR:HG23	1:A:369:ILE:HG21	1.81	0.63
1:A:285:ASN:HA	1:A:288:LYS:HG2	1.79	0.63
1:A:131:PHE:HA	1:A:135:LEU:HD23	1.81	0.63
1:A:203:TYR:CD2	1:A:261:GLU:HG2	2.34	0.63
1:A:319:GLU:OE2	1:A:320:VAL:HG23	1.98	0.63
1:A:438:ASP:OD2	1:A:440:GLU:HG2	1.99	0.63
1:A:153:LEU:HD11	1:A:160:ALA:HB1	1.81	0.63
1:A:113:ARG:H	1:A:169:ASP:HB2	1.64	0.62
1:A:378:LEU:O	1:A:382:GLN:HG3	2.00	0.62
1:A:100:ILE:HD12	1:A:100:ILE:C	2.20	0.62
1:A:122:THR:HG21	1:A:162:GLU:HB2	1.82	0.62
1:A:695:CYS:HA	1:A:728:VAL:C	2.20	0.62
1:A:285:ASN:HD22	1:A:288:LYS:HD3	1.64	0.61
1:A:349:ARG:NH2	1:A:561:GLU:CB	2.64	0.61
1:A:297:ALA:HA	1:A:298:PRO:C	2.21	0.60
1:A:192:GLU:HB3	1:A:194:GLU:OE2	2.01	0.60
1:A:197:SER:O	1:A:200:GLU:HG3	2.00	0.60
1:A:105:CYS:O	1:A:108:VAL:HG23	2.01	0.60
1:A:360:PHE:O	1:A:362:ARG:N	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:HH11	1:A:93:ARG:NH1	2.00	0.60
1:A:114:ILE:CD1	1:A:176:VAL:HG22	2.32	0.60
1:A:430:ILE:HG13	1:A:432:LEU:HD13	1.84	0.60
1:A:126:ILE:HD13	1:A:159:ARG:HD2	1.83	0.60
1:A:373:ASP:OD2	1:A:469:VAL:CB	2.50	0.60
1:A:169:ASP:O	1:A:171:SER:N	2.35	0.59
1:A:384:HIS:HE1	2:A:817:ADP:N3	1.99	0.59
1:A:27:ILE:HG12	1:A:80:GLU:OE1	2.02	0.59
1:A:65:ARG:HH11	1:A:93:ARG:HH12	1.48	0.58
1:A:430:ILE:CD1	1:A:432:LEU:HD13	2.33	0.58
1:A:318:GLY:C	1:A:320:VAL:H	2.08	0.58
1:A:324:ILE:O	1:A:327:GLN:HB3	2.03	0.58
1:A:360:PHE:O	1:A:364:ASP:HB3	2.04	0.57
1:A:183:HIS:HB3	1:A:185:GLU:OE2	2.05	0.57
1:A:227:PRO:HB3	1:A:339:ALA:HA	1.86	0.57
1:A:275:MET:HG3	1:A:308:ALA:O	2.04	0.57
1:A:201:VAL:HG12	1:A:257:ALA:HB2	1.87	0.57
1:A:53:ARG:O	1:A:72:LEU:HD23	2.05	0.57
1:A:383:ILE:O	1:A:386:LYS:HG2	2.04	0.56
1:A:431:ASP:C	1:A:432:LEU:HD12	2.26	0.56
1:A:431:ASP:O	1:A:432:LEU:HD12	2.05	0.56
1:A:38:VAL:HG21	1:A:72:LEU:HD12	1.87	0.56
1:A:311:PRO:O	1:A:313:ARG:N	2.38	0.56
1:A:129:ASN:C	1:A:129:ASN:ND2	2.54	0.56
1:A:312:LYS:HE2	1:A:354:ASP:OD2	2.05	0.56
1:A:297:ALA:HB2	1:A:341:VAL:HG12	1.88	0.56
1:A:146:ILE:HD12	1:A:165:VAL:HG11	1.86	0.55
1:A:233:ILE:HG23	1:A:235:VAL:H	1.71	0.55
1:A:414:LEU:HD21	1:A:456:LEU:CD2	2.36	0.55
1:A:347:THR:HG23	1:A:349:ARG:N	2.20	0.55
1:A:406:HIS:HD2	1:A:410:ASP:HB3	1.71	0.55
1:A:89:ARG:HG2	1:A:94:VAL:O	2.07	0.55
1:A:350:PRO:HB3	1:A:358:ARG:NH2	2.22	0.54
1:A:140:LEU:HG	1:A:141:GLU:HG3	1.88	0.54
1:A:336:LYS:N	1:A:336:LYS:HD3	2.22	0.54
1:A:389:LYS:HD3	1:A:446:ALA:HB2	1.87	0.54
1:A:408:GLY:HA3	2:A:817:ADP:C8	2.43	0.54
1:A:353:ILE:CG2	1:A:357:LEU:HD12	2.33	0.54
1:A:185:GLU:H	1:A:185:GLU:CD	2.10	0.53
1:A:302:PHE:HA	1:A:344:MET:O	2.07	0.53
1:A:285:ASN:O	1:A:288:LYS:HG2	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PHE:O	1:A:140:LEU:C	2.46	0.53
1:A:291:GLU:O	1:A:295:LYS:HG3	2.09	0.53
1:A:424:ARG:HA	1:A:428:ASP:HB2	1.90	0.53
1:A:249:THR:HG23	1:A:369:ILE:HG22	1.91	0.53
1:A:120:ASP:OD1	1:A:121:ASP:N	2.41	0.53
1:A:445:LEU:HD23	1:A:445:LEU:C	2.29	0.53
1:A:226:HIS:N	1:A:227:PRO:HD3	2.24	0.52
1:A:284:SER:O	1:A:287:ARG:HG2	2.09	0.52
1:A:405:GLY:HA3	1:A:463:ALA:HB3	1.90	0.52
1:A:91:ASN:ND2	1:A:151:ILE:H	2.03	0.52
1:A:414:LEU:HD21	1:A:456:LEU:HD21	1.91	0.52
1:A:164:LYS:HB3	1:A:189:ILE:HD11	1.91	0.52
1:A:100:ILE:HD12	1:A:100:ILE:O	2.09	0.52
1:A:230:PHE:HA	1:A:233:ILE:HG22	1.92	0.52
1:A:249:THR:CG2	1:A:369:ILE:CG2	2.87	0.52
1:A:292:GLU:HA	1:A:295:LYS:HE3	1.92	0.52
1:A:319:GLU:CD	1:A:320:VAL:HG23	2.30	0.52
1:A:358:ARG:O	1:A:359:ARG:C	2.48	0.52
1:A:426:LYS:O	1:A:427:MET:C	2.49	0.52
1:A:433:GLU:O	1:A:434:ASP:CG	2.48	0.52
1:A:192:GLU:O	1:A:195:GLU:N	2.42	0.51
1:A:53:ARG:NH1	1:A:72:LEU:HD22	2.26	0.51
1:A:129:ASN:HD21	1:A:131:PHE:HB3	1.75	0.51
1:A:209:CYS:C	1:A:210:ARG:HG3	2.30	0.51
1:A:312:LYS:O	1:A:316:THR:HG22	2.11	0.51
1:A:126:ILE:HG12	1:A:159:ARG:NH1	2.26	0.50
1:A:312:LYS:HA	1:A:316:THR:CG2	2.41	0.50
1:A:320:VAL:O	1:A:324:ILE:HG13	2.11	0.50
1:A:285:ASN:ND2	1:A:288:LYS:HD3	2.26	0.50
1:A:224:LEU:HD12	1:A:298:PRO:HB3	1.94	0.50
1:A:430:ILE:HG13	1:A:431:ASP:N	2.27	0.50
1:A:199:ASN:O	1:A:199:ASN:CG	2.50	0.50
1:A:265:PHE:CD2	1:A:296:ASN:HB2	2.47	0.50
1:A:60:LYS:HG2	1:A:66:GLU:HG2	1.92	0.49
1:A:243:LEU:HB3	1:A:251:LYS:HD3	1.93	0.49
1:A:292:GLU:HG3	1:A:295:LYS:HZ1	1.76	0.49
1:A:349:ARG:HB2	1:A:350:PRO:HD2	1.94	0.49
1:A:695:CYS:C	1:A:728:VAL:CB	2.78	0.49
1:A:56:THR:HG22	1:A:70:ILE:HD13	1.93	0.49
1:A:305:GLU:O	1:A:307:ASP:N	2.46	0.49
1:A:385:THR:HG22	1:A:388:MET:HE2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ALA:CB	1:A:357:LEU:HD11	2.44	0.48
1:A:209:CYS:O	1:A:210:ARG:HG3	2.13	0.48
1:A:695:CYS:CB	1:A:729:PRO:N	2.77	0.48
1:A:136:LYS:HB2	1:A:136:LYS:NZ	2.29	0.48
1:A:358:ARG:HG3	1:A:358:ARG:NH1	2.28	0.48
1:A:164:LYS:HG3	1:A:165:VAL:N	2.28	0.48
1:A:358:ARG:HH11	1:A:358:ARG:HG3	1.78	0.48
1:A:458:GLN:O	1:A:459:SER:O	2.32	0.48
1:A:56:THR:HG22	1:A:70:ILE:CD1	2.44	0.48
1:A:278:LEU:HG	1:A:281:GLU:OE1	2.14	0.47
1:A:27:ILE:HD13	1:A:99:VAL:CG1	2.35	0.47
1:A:251:LYS:HD2	1:A:346:ALA:HB1	1.96	0.47
1:A:364:ASP:OD1	1:A:365:ARG:HG2	2.14	0.47
1:A:285:ASN:ND2	1:A:288:LYS:NZ	2.62	0.47
1:A:40:SER:HB3	1:A:74:ASP:HB2	1.96	0.47
1:A:430:ILE:CG1	1:A:432:LEU:HD13	2.44	0.47
1:A:158:MET:CE	1:A:419:ALA:HB1	2.44	0.47
1:A:407:VAL:O	1:A:410:ASP:HB2	2.15	0.47
1:A:424:ARG:HA	1:A:428:ASP:CB	2.45	0.47
1:A:52:PHE:O	1:A:54:GLY:N	2.48	0.47
1:A:585:ALA:O	1:A:586:ARG:C	2.54	0.46
1:A:194:GLU:N	1:A:194:GLU:CD	2.59	0.46
1:A:219:MET:HE3	1:A:241:ILE:HD13	1.96	0.46
1:A:335:LEU:O	1:A:336:LYS:HE3	2.16	0.46
1:A:203:TYR:CD2	1:A:217:LYS:HE2	2.50	0.46
1:A:292:GLU:HG3	1:A:295:LYS:HZ2	1.79	0.46
1:A:347:THR:HG23	1:A:348:ASN:N	2.30	0.46
1:A:406:HIS:CD2	1:A:410:ASP:HB3	2.49	0.46
1:A:185:GLU:O	1:A:187:GLU:N	2.43	0.46
1:A:312:LYS:HE2	1:A:354:ASP:OD1	2.16	0.46
1:A:335:LEU:C	1:A:336:LYS:HD3	2.36	0.46
1:A:155:ARG:CZ	1:A:386:LYS:HD2	2.46	0.46
1:A:41:LEU:HD21	1:A:82:ILE:HD12	1.97	0.46
1:A:148:LYS:HG2	1:A:149:GLY:N	2.31	0.45
1:A:136:LYS:HB2	1:A:136:LYS:HZ3	1.81	0.45
1:A:325:VAL:O	1:A:328:LEU:N	2.49	0.45
1:A:312:LYS:HE2	1:A:354:ASP:CG	2.37	0.45
1:A:360:PHE:C	1:A:362:ARG:H	2.20	0.45
1:A:68:VAL:HG23	1:A:147:ARG:HB2	1.98	0.45
1:A:190:LYS:H	1:A:190:LYS:CD	2.19	0.45
1:A:695:CYS:CB	1:A:729:PRO:CA	2.94	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:O	1:A:262:THR:HG23	2.17	0.45
1:A:423:ILE:HA	1:A:445:LEU:HD11	1.98	0.44
1:A:28:VAL:HG12	1:A:98:ASP:O	2.17	0.44
1:A:117:LEU:HD12	1:A:189:ILE:HG23	1.99	0.44
1:A:270:ASN:HD22	1:A:304:ASP:HB3	1.83	0.44
1:A:65:ARG:NH1	1:A:93:ARG:HH12	2.15	0.44
1:A:53:ARG:CZ	1:A:72:LEU:HD22	2.48	0.44
1:A:239:ARG:NH1	1:A:336:LYS:NZ	2.66	0.44
1:A:241:ILE:HB	1:A:344:MET:HG2	2.00	0.44
1:A:329:LEU:HD23	1:A:357:LEU:HD23	1.99	0.43
1:A:284:SER:HA	1:A:287:ARG:NE	2.33	0.43
1:A:427:MET:O	1:A:430:ILE:CG1	2.48	0.43
1:A:26:LEU:HB3	1:A:80:GLU:O	2.18	0.43
1:A:353:ILE:CG2	1:A:354:ASP:N	2.81	0.43
1:A:114:ILE:HD11	1:A:176:VAL:HG22	2.01	0.43
1:A:335:LEU:O	1:A:336:LYS:CB	2.66	0.43
1:A:56:THR:HA	1:A:69:CYS:O	2.18	0.43
1:A:28:VAL:HA	1:A:82:ILE:HG23	2.00	0.43
1:A:244:TYR:CE2	1:A:350:PRO:HG3	2.54	0.42
1:A:220:VAL:HB	1:A:224:LEU:CD2	2.47	0.42
1:A:219:MET:CE	1:A:241:ILE:HD13	2.50	0.42
1:A:318:GLY:C	1:A:320:VAL:N	2.71	0.42
1:A:424:ARG:C	1:A:428:ASP:HB3	2.39	0.42
1:A:198:LEU:C	1:A:200:GLU:H	2.22	0.42
1:A:43:GLN:N	1:A:44:PRO:HD2	2.35	0.42
1:A:129:ASN:HD21	1:A:132:GLU:N	2.08	0.42
1:A:201:VAL:CG1	1:A:253:LEU:HD23	2.49	0.42
1:A:324:ILE:O	1:A:325:VAL:C	2.57	0.42
1:A:146:ILE:HG13	1:A:146:ILE:O	2.18	0.42
1:A:213:LEU:O	1:A:217:LYS:HG3	2.20	0.42
1:A:129:ASN:HD22	1:A:130:LEU:N	2.18	0.42
1:A:235:VAL:HG12	1:A:236:LYS:N	2.34	0.42
1:A:430:ILE:CG1	1:A:431:ASP:N	2.83	0.42
1:A:570:ALA:HA	1:A:571:PRO:C	2.40	0.42
1:A:131:PHE:HD1	1:A:135:LEU:HB2	1.84	0.42
1:A:377:ARG:NH2	1:A:467:THR:O	2.53	0.42
1:A:374:ALA:H	1:A:469:VAL:N	2.18	0.41
1:A:249:THR:CG2	1:A:369:ILE:HG21	2.48	0.41
1:A:408:GLY:HA3	2:A:817:ADP:N7	2.36	0.41
1:A:436:THR:O	1:A:436:THR:HG23	2.20	0.41
1:A:148:LYS:HE2	1:A:166:VAL:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLU:HG2	1:A:34:GLU:O	2.21	0.41
1:A:373:ASP:OD1	1:A:376:GLY:N	2.40	0.41
1:A:312:LYS:O	1:A:313:ARG:C	2.58	0.41
1:A:112:LYS:H	1:A:170:PRO:HD3	1.85	0.41
1:A:238:PRO:HB3	1:A:365:ARG:HH11	1.85	0.41
1:A:315:LYS:O	1:A:315:LYS:HG3	2.19	0.41
1:A:38:VAL:HG22	1:A:39:VAL:N	2.35	0.41
1:A:328:LEU:O	1:A:332:MET:HG2	2.21	0.41
1:A:91:ASN:HD21	1:A:151:ILE:N	2.06	0.41
1:A:132:GLU:O	1:A:137:PRO:HD3	2.21	0.40
1:A:158:MET:HE1	1:A:419:ALA:HB1	2.03	0.40
1:A:229:LEU:O	1:A:233:ILE:HB	2.21	0.40
1:A:306:LEU:HD23	1:A:353:ILE:CD1	2.52	0.40
1:A:152:PHE:CZ	1:A:163:PHE:HB2	2.55	0.40
1:A:254:ILE:CD1	1:A:369:ILE:HD11	2.51	0.40
1:A:206:VAL:CG2	1:A:253:LEU:HD22	2.44	0.40

All (8) 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:321:GLU:OE2	1:A:322:ARG:NE[5_665]	1.65	0.55
1:A:321:GLU:OE2	1:A:322:ARG:CD[5_665]	1.72	0.48
1:A:549:THR:CB	1:A:599:ARG:CB[5_665]	1.83	0.37
1:A:275:MET:CE	1:A:322:ARG:NH1[5_665]	1.95	0.25
1:A:549:THR:CA	1:A:599:ARG:CB[5_665]	2.00	0.20
1:A:398:GLN:NE2	1:A:504:LEU:O[5_665]	2.10	0.10
1:A:226:HIS:ND1	1:A:434:ASP:OD1[6_545]	2.15	0.05
1:A:125:GLY:O	1:A:232:ALA:CB[5_665]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	673/816 (82%)	566 (84%)	64 (10%)	43 (6%)	1	21

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	186	GLY
1	A	306	LEU
1	A	312	LYS
1	A	360	PHE
1	A	426	LYS
1	A	459	SER
1	A	460	ASN
1	A	471	VAL
1	A	487	ARG
1	A	586	ARG
1	A	626	PRO
1	A	646	PRO
1	A	647	LEU
1	A	140	LEU
1	A	141	GLU
1	A	185	GLU
1	A	304	ASP
1	A	313	ARG
1	A	335	LEU
1	A	351	ASN
1	A	361	GLY
1	A	404	HIS
1	A	436	THR
1	A	590	ILE
1	A	637	GLY
1	A	193	ASP
1	A	311	PRO
1	A	319	GLU
1	A	359	ARG
1	A	435	GLU
1	A	472	PRO
1	A	474	VAL
1	A	585	ALA
1	A	636	PRO
1	A	639	LEU
1	A	473	GLN
1	A	475	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	350	PRO
1	A	427	MET
1	A	482	LEU
1	A	437	ILE
1	A	169	ASP

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	382/686 (56%)	357 (94%)	25 (6%)	20 59

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	22	ARG
1	A	28	VAL
1	A	45	LYS
1	A	109	LYS
1	A	112	LYS
1	A	114	ILE
1	A	129	ASN
1	A	136	LYS
1	A	147	ARG
1	A	155	ARG
1	A	164	LYS
1	A	190	LYS
1	A	194	GLU
1	A	212	GLN
1	A	224	LEU
1	A	243	LEU
1	A	249	THR
1	A	273	GLU
1	A	314	GLU
1	A	319	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	336	LYS
1	A	340	HIS
1	A	341	VAL
1	A	347	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	90	ASN
1	A	91	ASN
1	A	103	GLN
1	A	129	ASN
1	A	285	ASN
1	A	340	HIS
1	A	348	ASN
1	A	384	HIS
1	A	406	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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
2	ADP	A	817	-	25,29,29	1.26	3 (12%)	24,45,45	1.74	3 (12%)

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
2	ADP	A	817	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	817	ADP	C4-N3	-3.21	1.30	1.35
2	A	817	ADP	C5-C4	-2.19	1.35	1.40
2	A	817	ADP	PB-O3A	2.34	1.63	1.60

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	817	ADP	N3-C2-N1	-6.67	123.05	128.86
2	A	817	ADP	C5'-C4'-C3'	-2.32	106.45	115.29
2	A	817	ADP	C4'-O4'-C1'	2.23	112.14	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	817	ADP	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	27:ILE	C	28:VAL	N	1.19
1	A	477:GLU	C	478:ASP	N	0.95

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.