



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:18 PM UTC

PDB ID : 3PIH / pdb_00003pih
Title : T. maritima UvrA in complex with fluorescein-modified DNA
Authors : Jaciuk, M.; Nowak, E.; Nowotny, M.
Deposited on : 2010-11-06
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

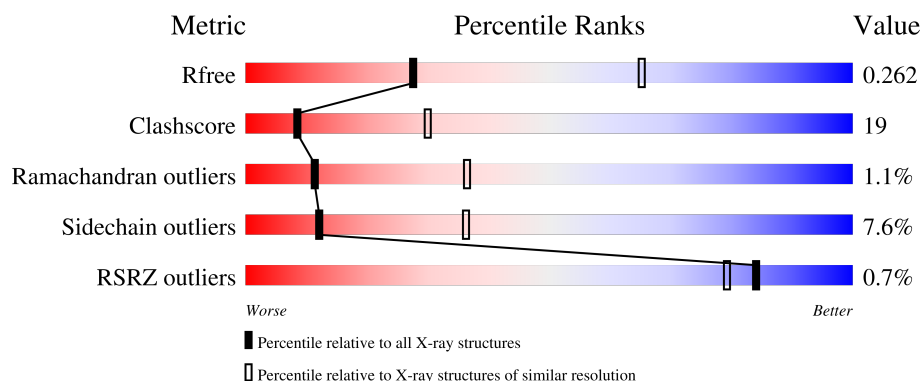
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

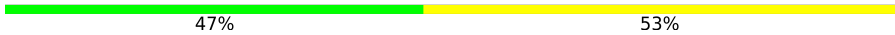
The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	916	
2	D	32	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7093 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.

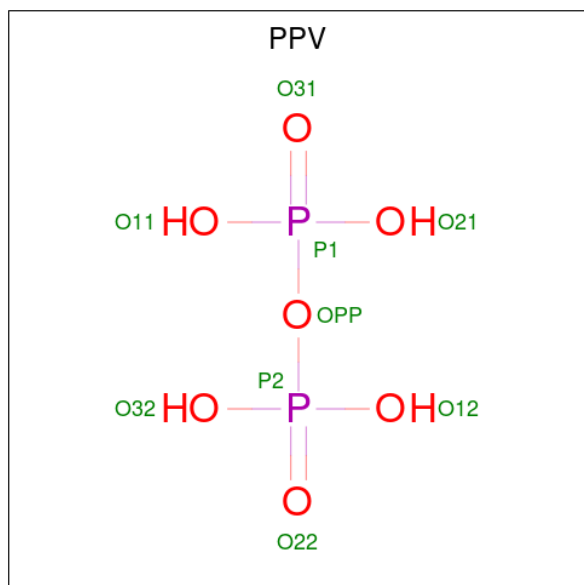
- Molecule 1 is a protein called UvrABC system protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	0	0	0
			6395	4030	1126	1217	22			

- Molecule 2 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	32	Total	C	N	O	P	0	0	0
			653	312	120	190	31			

- Molecule 3 is PYROPHOSPHATE (CCD ID: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			9	7	2		
3	A	1	Total	O	P	0	0
			9	7	2		

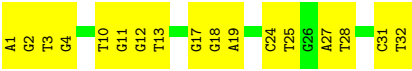
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total 22	O 22	0	0
5	D	2	Total 2	O 2	0	0

● Molecule 2: DNA (32-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	107.51Å 107.51Å 108.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.08 – 2.90 48.08 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.5 (48.08-2.90) 96.0 (48.08-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.198 , 0.265 0.198 , 0.262	Depositor DCC
R_{free} test set	1312 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k 0.005 for -h,l,k 0.004 for l,-k,h 0.017 for -l,-k,-h 0.049 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7093	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.43	0/6499	0.85	10/8797 (0.1%)
2	D	0.27	0/732	0.87	0/1128
All	All	0.42	0/7231	0.85	10/9925 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	ASN	CA-C-N	6.59	127.16	120.04
1	A	561	ASN	C-N-CA	6.59	127.16	120.04
1	A	779	ILE	CA-C-N	6.44	125.94	119.24
1	A	779	ILE	C-N-CA	6.44	125.94	119.24
1	A	587	TYR	N-CA-C	-6.24	106.26	114.31
1	A	291	SER	N-CA-C	-5.94	105.86	112.57
1	A	276	CYS	CA-C-N	5.67	125.14	119.24
1	A	276	CYS	C-N-CA	5.67	125.14	119.24
1	A	445	LEU	N-CA-C	-5.14	105.86	111.82
1	A	875	ASP	N-CA-C	-5.07	107.22	113.41

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	6395	0	6295	238	0
2	D	653	0	362	23	0
3	A	18	0	0	1	0
4	A	3	0	0	0	0
5	A	22	0	0	2	0
5	D	2	0	0	0	0
All	All	7093	0	6657	261	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 19.

All (261) 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:369:GLU:N	1:A:370:MET:HA	1.84	0.92
2:D:3:DT:H2'	2:D:4:DG:C8	2.07	0.89
1:A:583:ARG:HH11	1:A:897:PRO:HG2	1.35	0.87
1:A:794:LEU:O	1:A:797:VAL:HG23	1.80	0.81
1:A:208:LEU:HD12	1:A:214:ASN:HD22	1.45	0.80
1:A:669:ILE:HD11	1:A:815:LYS:HB2	1.64	0.80
1:A:35:SER:HB2	1:A:538:ILE:HG22	1.63	0.78
1:A:328:SER:HB2	1:A:329:PRO:HA	1.66	0.77
1:A:901:ALA:O	1:A:913:LYS:HE3	1.85	0.76
1:A:854:LEU:O	1:A:859:ASN:HB2	1.87	0.74
1:A:87:GLN:HE21	1:A:495:ILE:HD12	1.52	0.74
1:A:340:VAL:HG13	1:A:340:VAL:O	1.88	0.73
1:A:414:ILE:HD11	1:A:449:VAL:HG23	1.70	0.73
1:A:633:PRO:HB2	1:A:646:ALA:HB2	1.70	0.73
1:A:461:SER:OG	1:A:463:THR:HB	1.90	0.71
1:A:729:MET:HB2	1:A:732:LEU:HD11	1.72	0.71
1:A:813:ARG:HD3	1:A:839:LEU:HD21	1.71	0.71
2:D:12:DG:H1'	2:D:13:DT:H5'	1.72	0.71
2:D:18:DG:H5'	2:D:18:DG:C8	2.27	0.70
1:A:87:GLN:HE21	1:A:495:ILE:CD1	2.06	0.69
1:A:289:ASP:HB2	1:A:380:VAL:HG12	1.74	0.69
2:D:18:DG:H2''	2:D:19:DA:C8	2.27	0.68
1:A:583:ARG:NH1	1:A:897:PRO:HG2	2.08	0.68
2:D:31:DC:H2'	2:D:32:DT:C6	2.28	0.68
1:A:868:LEU:O	1:A:872:LYS:HG3	1.93	0.68
1:A:794:LEU:HG	1:A:797:VAL:HG21	1.75	0.67
1:A:355:VAL:HB	1:A:356:PRO:HD3	1.77	0.66
1:A:412:LEU:HB3	1:A:416:GLU:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ASP:O	1:A:529:ILE:HG13	1.97	0.65
1:A:586:PRO:HG3	1:A:608:PRO:HB3	1.79	0.65
1:A:87:GLN:NE2	1:A:495:ILE:HD12	2.12	0.65
1:A:342:GLU:O	1:A:346:TYR:HD2	1.80	0.65
1:A:438:LEU:O	1:A:442:GLU:HG3	1.97	0.65
1:A:152:LEU:HB2	1:A:234:GLU:HB3	1.79	0.64
1:A:414:ILE:HD11	1:A:449:VAL:CG2	2.28	0.64
1:A:806:LEU:HD21	1:A:814:ILE:HD12	1.80	0.64
1:A:562:PRO:C	1:A:564:SER:H	2.05	0.63
1:A:209:ILE:HG22	1:A:211:GLU:HG3	1.81	0.62
1:A:498:HIS:ND1	1:A:499:PRO:HD2	2.15	0.61
2:D:12:DG:H1'	2:D:13:DT:C5'	2.30	0.61
1:A:583:ARG:NH1	1:A:872:LYS:O	2.34	0.61
2:D:11:DG:H2''	2:D:12:DG:H5'	1.83	0.61
1:A:237:ASN:C	1:A:237:ASN:HD22	2.07	0.61
1:A:397:LEU:HA	1:A:405:ASN:HD22	1.66	0.61
1:A:756:TYR:CE2	1:A:757:LYS:HG3	2.36	0.60
1:A:69:LYS:O	1:A:71:PRO:HD3	2.01	0.60
2:D:12:DG:H2''	2:D:13:DT:OP2	2.00	0.60
1:A:110:VAL:HG12	1:A:437:LEU:HD11	1.83	0.60
2:D:31:DC:H3'	2:D:32:DT:H72	1.83	0.60
1:A:371:LYS:O	1:A:375:GLU:HG2	2.02	0.60
1:A:745:LYS:O	1:A:746:ARG:HG2	2.00	0.60
1:A:779:ILE:N	1:A:779:ILE:HD12	2.17	0.60
1:A:812:GLN:HG2	5:A:938:HOH:O	2.01	0.58
1:A:690:LEU:C	1:A:690:LEU:HD23	2.28	0.58
1:A:121:PRO:HD2	1:A:257:ILE:HD11	1.84	0.58
1:A:88:LYS:O	1:A:89:THR:C	2.47	0.58
1:A:566:LEU:HD21	1:A:842:GLU:HB2	1.86	0.58
1:A:791:ASP:O	1:A:846:LYS:HB3	2.03	0.58
1:A:120:CYS:HB3	1:A:123:CYS:SG	2.42	0.57
1:A:402:ASN:ND2	1:A:424:LEU:HD12	2.19	0.57
1:A:344:ILE:O	1:A:354:VAL:HG23	2.05	0.57
1:A:444:ARG:HA	1:A:447:PHE:CD2	2.39	0.57
2:D:17:DG:H1'	2:D:18:DG:H5'	1.85	0.57
1:A:104:ILE:HD13	1:A:445:LEU:HD12	1.87	0.56
1:A:623:LYS:HG3	3:A:1001:PPV:O21	2.05	0.56
1:A:414:ILE:CG1	1:A:454:GLU:HA	2.36	0.56
1:A:579:VAL:O	1:A:580:ASN:C	2.48	0.56
1:A:245:ILE:N	1:A:245:ILE:HD12	2.21	0.55
1:A:418:LEU:HG	1:A:445:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LYS:HB3	1:A:538:ILE:HB	1.87	0.55
1:A:307:PRO:HB3	1:A:378:PHE:CE2	2.41	0.54
1:A:387:CYS:O	1:A:390:ARG:HG3	2.07	0.54
1:A:87:GLN:O	1:A:88:LYS:HD2	2.08	0.54
1:A:440:GLU:O	1:A:443:LYS:HG2	2.08	0.54
1:A:676:ASN:ND2	1:A:800:GLY:HA2	2.22	0.54
1:A:132:ILE:HD12	1:A:219:LEU:HD22	1.89	0.54
1:A:500:ARG:HD3	1:A:501:ASP:OD1	2.08	0.54
1:A:726:LYS:NZ	1:A:726:LYS:HB3	2.23	0.53
1:A:798:LYS:O	1:A:801:GLN:HB2	2.08	0.53
1:A:671:ARG:NH1	1:A:806:LEU:O	2.41	0.53
1:A:697:ALA:HB2	1:A:754:ILE:HG21	1.90	0.53
1:A:15:LYS:HG2	1:A:548:ARG:HH11	1.73	0.53
2:D:1:DA:O5'	2:D:1:DA:H8	1.91	0.53
1:A:903:ASN:OD1	1:A:905:HIS:HB2	2.08	0.53
1:A:429:ARG:O	1:A:429:ARG:HD3	2.10	0.52
1:A:562:PRO:C	1:A:564:SER:N	2.67	0.52
1:A:660:LYS:CB	1:A:828:THR:HG22	2.38	0.52
2:D:2:DG:C8	2:D:3:DT:H72	2.44	0.52
1:A:809:GLY:O	1:A:813:ARG:HB2	2.09	0.52
1:A:601:LYS:HG3	1:A:890:TYR:CZ	2.44	0.52
1:A:543:GLY:N	1:A:796:TYR:CE1	2.78	0.52
1:A:632:TYR:HB3	1:A:633:PRO:HD3	1.90	0.52
1:A:281:GLY:HA2	1:A:391:ARG:O	2.10	0.52
1:A:442:GLU:O	1:A:446:GLU:HG3	2.09	0.52
2:D:10:DT:H2''	2:D:11:DG:C8	2.45	0.52
1:A:135:ILE:O	1:A:139:LEU:HG	2.10	0.52
1:A:690:LEU:HD21	1:A:756:TYR:CD1	2.45	0.52
1:A:803:ALA:O	1:A:806:LEU:HB2	2.10	0.52
1:A:743:LYS:HG2	1:A:743:LYS:O	2.11	0.51
1:A:416:GLU:O	1:A:419:GLU:HG3	2.10	0.51
1:A:289:ASP:C	1:A:291:SER:H	2.18	0.51
1:A:269:PHE:HB3	1:A:392:LEU:HD23	1.92	0.51
1:A:281:GLY:O	1:A:391:ARG:HD3	2.10	0.51
1:A:422:LYS:C	1:A:424:LEU:H	2.19	0.51
1:A:708:SER:HB3	1:A:711:LEU:HD12	1.92	0.51
1:A:308:TYR:OH	1:A:357:LYS:HD2	2.11	0.51
1:A:289:ASP:HB2	1:A:380:VAL:CG1	2.41	0.50
1:A:339:ASP:O	1:A:340:VAL:HB	2.11	0.50
1:A:825:THR:OG1	1:A:828:THR:HG23	2.10	0.50
1:A:97:THR:OG1	1:A:100:THR:HG23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LYS:HE2	1:A:888:GLY:O	2.11	0.50
2:D:10:DT:H2''	2:D:11:DG:H8	1.76	0.50
1:A:676:ASN:HB2	1:A:677:PRO:HD2	1.92	0.50
1:A:769:VAL:HB	1:A:795:GLY:HA2	1.93	0.50
2:D:12:DG:H5'	2:D:12:DG:C8	2.47	0.50
1:A:498:HIS:CG	1:A:499:PRO:HD2	2.47	0.50
1:A:745:LYS:C	1:A:746:ARG:HG2	2.37	0.50
1:A:34:GLY:HA3	1:A:796:TYR:OH	2.11	0.49
1:A:35:SER:CB	1:A:538:ILE:HG22	2.39	0.49
1:A:700:ARG:HD2	1:A:702:TYR:CE1	2.47	0.49
1:A:95:ARG:HD3	1:A:270:ASN:OD1	2.13	0.49
1:A:381:GLN:O	1:A:381:GLN:HG3	2.12	0.49
1:A:794:LEU:HD22	1:A:813:ARG:HB3	1.94	0.49
1:A:208:LEU:HD12	1:A:214:ASN:ND2	2.21	0.49
1:A:716:CYS:SG	1:A:742:CYS:HB3	2.53	0.49
2:D:18:DG:C2'	2:D:19:DA:C8	2.95	0.49
1:A:87:GLN:H	1:A:87:GLN:CD	2.17	0.48
1:A:414:ILE:HG13	1:A:454:GLU:HA	1.95	0.48
1:A:608:PRO:HB2	1:A:611:VAL:CG2	2.44	0.48
1:A:729:MET:HB2	1:A:732:LEU:CD1	2.43	0.48
1:A:32:VAL:HA	1:A:840:HIS:CB	2.43	0.48
1:A:909:GLY:O	1:A:913:LYS:HG3	2.12	0.48
1:A:207:ARG:O	1:A:207:ARG:HG2	2.13	0.48
1:A:616:THR:HG21	1:A:871:ILE:HD13	1.95	0.48
1:A:696:ALA:O	1:A:700:ARG:HG3	2.14	0.47
1:A:835:PRO:HD2	1:A:865:GLU:HG2	1.96	0.47
1:A:15:LYS:HE2	1:A:548:ARG:HH12	1.78	0.47
1:A:59:THR:HG21	5:A:932:HOH:O	2.14	0.47
1:A:767:MET:HB2	1:A:771:GLU:HB3	1.95	0.47
1:A:7:LYS:O	1:A:74:ASP:HB2	2.14	0.47
1:A:549:VAL:HG11	1:A:552:GLN:NE2	2.30	0.47
1:A:150:TYR:CD2	1:A:207:ARG:HB2	2.50	0.47
1:A:413:SER:HA	1:A:456:LEU:O	2.14	0.47
1:A:434:VAL:O	1:A:435:GLY:C	2.58	0.47
1:A:830:TYR:HB2	1:A:861:VAL:HG22	1.97	0.47
1:A:234:GLU:O	1:A:235:ILE:HD13	2.15	0.47
1:A:341:LYS:H	1:A:341:LYS:HG2	1.34	0.47
1:A:87:GLN:NE2	1:A:495:ILE:CD1	2.73	0.47
1:A:260:PRO:CG	1:A:395:GLU:HG2	2.45	0.46
1:A:718:ALA:HB2	1:A:741:VAL:HG21	1.96	0.46
1:A:31:GLY:N	1:A:37:LYS:HE3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ARG:HH11	1:A:845:ARG:NH2	2.13	0.46
2:D:3:DT:C2'	2:D:4:DG:C8	2.91	0.46
2:D:18:DG:C8	2:D:18:DG:C5'	2.98	0.46
1:A:213:ARG:O	1:A:213:ARG:HG2	2.14	0.46
1:A:225:ALA:HB1	1:A:233:VAL:HG23	1.98	0.46
1:A:214:ASN:O	1:A:218:ILE:HG13	2.15	0.46
1:A:397:LEU:CA	1:A:405:ASN:HD22	2.29	0.46
1:A:634:ALA:HB1	1:A:652:ILE:HD11	1.98	0.46
1:A:896:THR:OG1	1:A:899:GLU:HG3	2.14	0.46
2:D:18:DG:H2'	2:D:19:DA:H8	1.79	0.46
1:A:268:SER:O	1:A:274:GLY:HA3	2.16	0.46
1:A:601:LYS:O	1:A:602:ASN:C	2.58	0.46
1:A:328:SER:HB2	1:A:329:PRO:CA	2.44	0.46
1:A:476:ALA:HA	1:A:479:ILE:HG22	1.98	0.46
1:A:71:PRO:O	1:A:73:VAL:HG23	2.15	0.46
1:A:492:GLU:OE2	1:A:838:GLY:N	2.48	0.46
1:A:5:VAL:HG22	1:A:20:ARG:HG2	1.98	0.45
1:A:307:PRO:HB3	1:A:378:PHE:CD2	2.51	0.45
1:A:500:ARG:O	1:A:500:ARG:HG2	2.14	0.45
1:A:535:ILE:O	1:A:552:GLN:HA	2.16	0.45
1:A:32:VAL:HA	1:A:840:HIS:HB2	1.98	0.45
1:A:226:MET:SD	1:A:248:GLU:HB3	2.56	0.45
1:A:340:VAL:O	1:A:340:VAL:CG1	2.58	0.45
1:A:612:PHE:C	1:A:612:PHE:HD2	2.24	0.45
1:A:709:PHE:C	1:A:709:PHE:CD2	2.94	0.45
1:A:562:PRO:O	1:A:564:SER:N	2.50	0.45
1:A:15:LYS:HB2	1:A:547:GLY:O	2.17	0.45
1:A:449:VAL:HG22	1:A:454:GLU:HB3	1.98	0.45
1:A:728:GLU:HG2	1:A:734:ASP:OD1	2.17	0.44
1:A:798:LYS:HE2	1:A:798:LYS:HB3	1.73	0.44
1:A:37:LYS:H	1:A:37:LYS:HG3	1.64	0.44
1:A:407:HIS:O	1:A:408:GLU:C	2.60	0.44
1:A:527:GLU:O	1:A:531:ASN:ND2	2.47	0.44
1:A:612:PHE:C	1:A:612:PHE:CD2	2.94	0.44
1:A:48:GLU:OE1	1:A:48:GLU:HA	2.17	0.44
1:A:120:CYS:CB	1:A:123:CYS:SG	3.05	0.44
1:A:500:ARG:HA	1:A:911:PHE:CZ	2.53	0.44
1:A:51:ARG:HH11	1:A:70:LYS:HA	1.83	0.44
1:A:342:GLU:O	1:A:346:TYR:CD2	2.67	0.44
1:A:806:LEU:HD21	1:A:814:ILE:CD1	2.47	0.44
1:A:616:THR:C	1:A:623:LYS:HD3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PRO:HB2	1:A:282:LEU:HD22	2.00	0.44
1:A:743:LYS:HE3	1:A:745:LYS:HG3	1.98	0.44
1:A:21:ILE:HA	1:A:22:PRO:HD3	1.90	0.43
1:A:608:PRO:HB2	1:A:611:VAL:HG21	2.01	0.43
1:A:614:CYS:SG	1:A:863:VAL:HG22	2.58	0.43
1:A:867:ASN:O	1:A:871:ILE:HG13	2.17	0.43
1:A:551:PHE:CZ	1:A:558:LEU:HB2	2.54	0.43
1:A:566:LEU:O	1:A:570:TYR:HD1	2.02	0.43
1:A:700:ARG:HD2	1:A:702:TYR:CZ	2.54	0.43
1:A:523:GLU:HG3	1:A:525:ASP:H	1.84	0.43
1:A:721:GLY:O	1:A:746:ARG:HB2	2.19	0.43
1:A:794:LEU:HD12	1:A:794:LEU:HA	1.83	0.43
1:A:833:ASP:O	1:A:834:GLU:C	2.61	0.43
1:A:749:ARG:O	1:A:753:GLU:HG3	2.19	0.43
2:D:27:DA:H2'	2:D:28:DT:C6	2.53	0.42
1:A:276:CYS:SG	1:A:277:PRO:HD2	2.59	0.42
1:A:414:ILE:HG12	1:A:454:GLU:HA	2.02	0.42
1:A:583:ARG:HG3	1:A:875:ASP:HA	2.00	0.42
1:A:208:LEU:N	1:A:208:LEU:HD23	2.35	0.42
1:A:14:LEU:HD21	1:A:40:LEU:HB2	2.00	0.42
1:A:697:ALA:HB1	1:A:702:TYR:HB2	2.02	0.42
1:A:3:GLU:HB2	1:A:21:ILE:O	2.19	0.42
1:A:15:LYS:HG2	1:A:548:ARG:NH1	2.34	0.42
1:A:343:PHE:O	1:A:344:ILE:C	2.61	0.42
1:A:374:LEU:HD12	1:A:374:LEU:N	2.35	0.42
2:D:24:DC:H2''	2:D:25:DT:O5'	2.19	0.42
1:A:120:CYS:SG	1:A:257:ILE:HD11	2.60	0.42
1:A:511:LYS:HB2	1:A:511:LYS:HE3	1.72	0.42
1:A:523:GLU:HG3	1:A:524:HIS:N	2.35	0.42
1:A:630:THR:O	1:A:633:PRO:HD2	2.20	0.42
2:D:24:DC:C6	2:D:25:DT:H72	2.54	0.42
1:A:834:GLU:O	1:A:837:VAL:HG23	2.20	0.41
1:A:97:THR:HB	1:A:458:LEU:O	2.20	0.41
1:A:813:ARG:CD	1:A:839:LEU:HD21	2.44	0.41
1:A:10:ARG:NH2	1:A:74:ASP:OD1	2.38	0.41
1:A:225:ALA:CB	1:A:233:VAL:HG23	2.50	0.41
1:A:702:TYR:N	1:A:702:TYR:CD2	2.88	0.41
1:A:276:CYS:HA	1:A:277:PRO:HD3	1.91	0.41
1:A:750:GLU:H	1:A:750:GLU:CD	2.28	0.41
1:A:806:LEU:HD12	1:A:806:LEU:HA	1.82	0.41
1:A:836:THR:HG21	1:A:870:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:DC:H2'	2:D:25:DT:H72	2.02	0.41
1:A:80:SER:O	1:A:81:PRO:C	2.64	0.41
1:A:649:PHE:HE1	1:A:652:ILE:HG13	1.85	0.41
1:A:724:TYR:O	1:A:724:TYR:CD1	2.73	0.41
1:A:206:ASP:OD1	1:A:208:LEU:HD22	2.21	0.41
1:A:289:ASP:O	1:A:291:SER:N	2.45	0.41
1:A:779:ILE:HD12	1:A:779:ILE:H	1.85	0.41
1:A:131:SER:OG	1:A:134:GLU:HG3	2.21	0.41
1:A:259:PHE:HA	1:A:260:PRO:HD3	1.89	0.41
1:A:340:VAL:C	1:A:342:GLU:N	2.78	0.41
1:A:430:GLU:C	1:A:432:GLU:H	2.28	0.41
1:A:500:ARG:HB2	1:A:911:PHE:CE2	2.56	0.41
1:A:11:VAL:O	1:A:14:LEU:HB2	2.20	0.40
1:A:150:TYR:CE2	1:A:207:ARG:HB2	2.56	0.40
1:A:893:ALA:C	1:A:894:THR:HG23	2.47	0.40
1:A:900:ILE:HG22	1:A:912:LEU:HD23	2.03	0.40
1:A:46:TYR:CD1	1:A:84:ALA:HB2	2.56	0.40
1:A:304:ALA:N	1:A:309:ARG:HE	2.19	0.40
1:A:339:ASP:O	1:A:340:VAL:CB	2.69	0.40
1:A:418:LEU:O	1:A:422:LYS:HD3	2.20	0.40
1:A:586:PRO:HA	1:A:609:LEU:O	2.21	0.40
1:A:749:ARG:HG2	1:A:750:GLU:N	2.35	0.40
1:A:108:LEU:HA	1:A:108:LEU:HD23	1.83	0.40
1:A:816:LEU:HG	1:A:820:LEU:HD12	2.04	0.40
1:A:821:ARG:C	1:A:821:ARG:HD2	2.47	0.40
1:A:252:CYS:HA	1:A:253:PRO:HD3	1.86	0.40
1:A:306:ILE:N	1:A:307:PRO:CD	2.85	0.40
1:A:726:LYS:HB3	1:A:726:LYS:HZ2	1.86	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	820/916 (90%)	739 (90%)	72 (9%)	9 (1%)	11	36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	VAL
1	A	435	GLY
1	A	775	PHE
1	A	72	ASP
1	A	540	PRO
1	A	563	ASP
1	A	757	LYS
1	A	290	PRO
1	A	121	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	681/803 (85%)	629 (92%)	52 (8%)	12	36

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	37	LYS
1	A	73	VAL
1	A	89	THR
1	A	92	HIS
1	A	142	SER
1	A	144	LYS
1	A	209	ILE
1	A	279	CYS
1	A	318	VAL
1	A	320	ARG
1	A	325	ARG

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Mol	Chain	Res	Type
1	A	340	VAL
1	A	341	LYS
1	A	385	SER
1	A	414	ILE
1	A	418	LEU
1	A	419	GLU
1	A	427	THR
1	A	429	ARG
1	A	437	LEU
1	A	451	VAL
1	A	463	THR
1	A	478	GLN
1	A	500	ARG
1	A	550	VAL
1	A	577	ILE
1	A	580	ASN
1	A	582	THR
1	A	590	LEU
1	A	605	VAL
1	A	624	SER
1	A	628	MET
1	A	656	GLU
1	A	698	LYS
1	A	726	LYS
1	A	730	LEU
1	A	749	ARG
1	A	762	SER
1	A	794	LEU
1	A	797	VAL
1	A	798	LYS
1	A	806	LEU
1	A	807	SER
1	A	813	ARG
1	A	827	ARG
1	A	845	ARG
1	A	855	VAL
1	A	863	VAL
1	A	900	ILE
1	A	906	SER
1	A	914	ASN

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

Mol	Chain	Res	Type
1	A	2	ASN
1	A	214	ASN
1	A	216	HIS
1	A	237	ASN
1	A	362	HIS
1	A	402	ASN
1	A	580	ASN
1	A	657	ASN
1	A	812	GLN
1	A	914	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	PPV	A	1001	-	6,8,8	0.99	1 (16%)	12,13,13	0.99	0
3	PPV	A	1002	-	6,8,8	0.98	0	12,13,13	1.06	1 (8%)

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	PPV	A	1001	-	-	0/6/6/6	-
3	PPV	A	1002	-	-	1/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	PPV	P2-O22	2.13	1.57	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	PPV	O21-P1-OPP	2.23	112.10	104.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	PPV	P2-OPP-P1-O11

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	PPV	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	836/916 (91%)	-0.27	6 (0%) 84 79	30, 61, 96, 114	0
2	D	32/32 (100%)	-0.37	0 100 100	46, 76, 89, 108	0
All	All	868/948 (91%)	-0.27	6 (0%) 84 79	30, 62, 96, 114	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	TYR	3.7
1	A	337	PRO	3.5
1	A	340	VAL	2.7
1	A	58	SER	2.5
1	A	348	ASP	2.4
1	A	322	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PPV	A	1002	9/9	0.94	0.14	52,67,81,94	0
3	PPV	A	1001	9/9	0.96	0.09	46,51,103,119	0
4	ZN	A	917	1/1	0.99	0.04	68,68,68,68	0
4	ZN	A	918	1/1	0.99	0.04	70,70,70,70	0
4	ZN	A	919	1/1	1.00	0.04	80,80,80,80	1

6.5 Other polymers [i](#)

There are no such residues in this entry.