



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:36 AM GMT

PDB ID : 3PIH
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

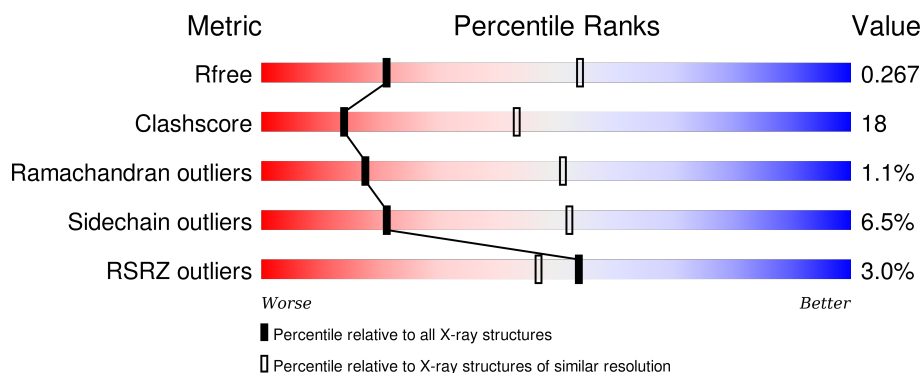
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 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.

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.

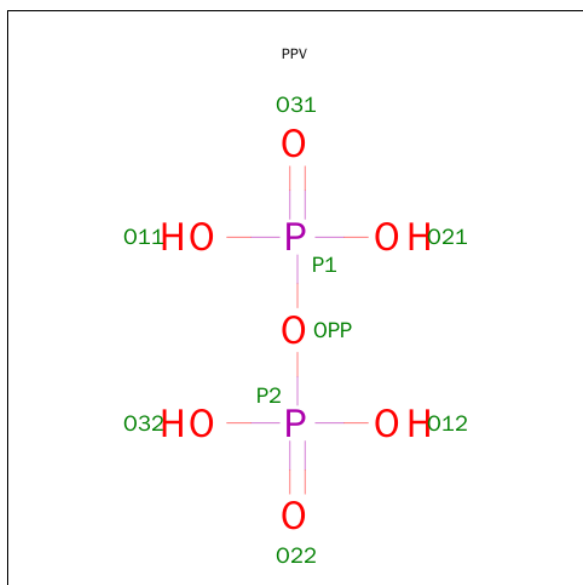
- Molecule 1 is a protein called UvrABC system protein A.

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

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

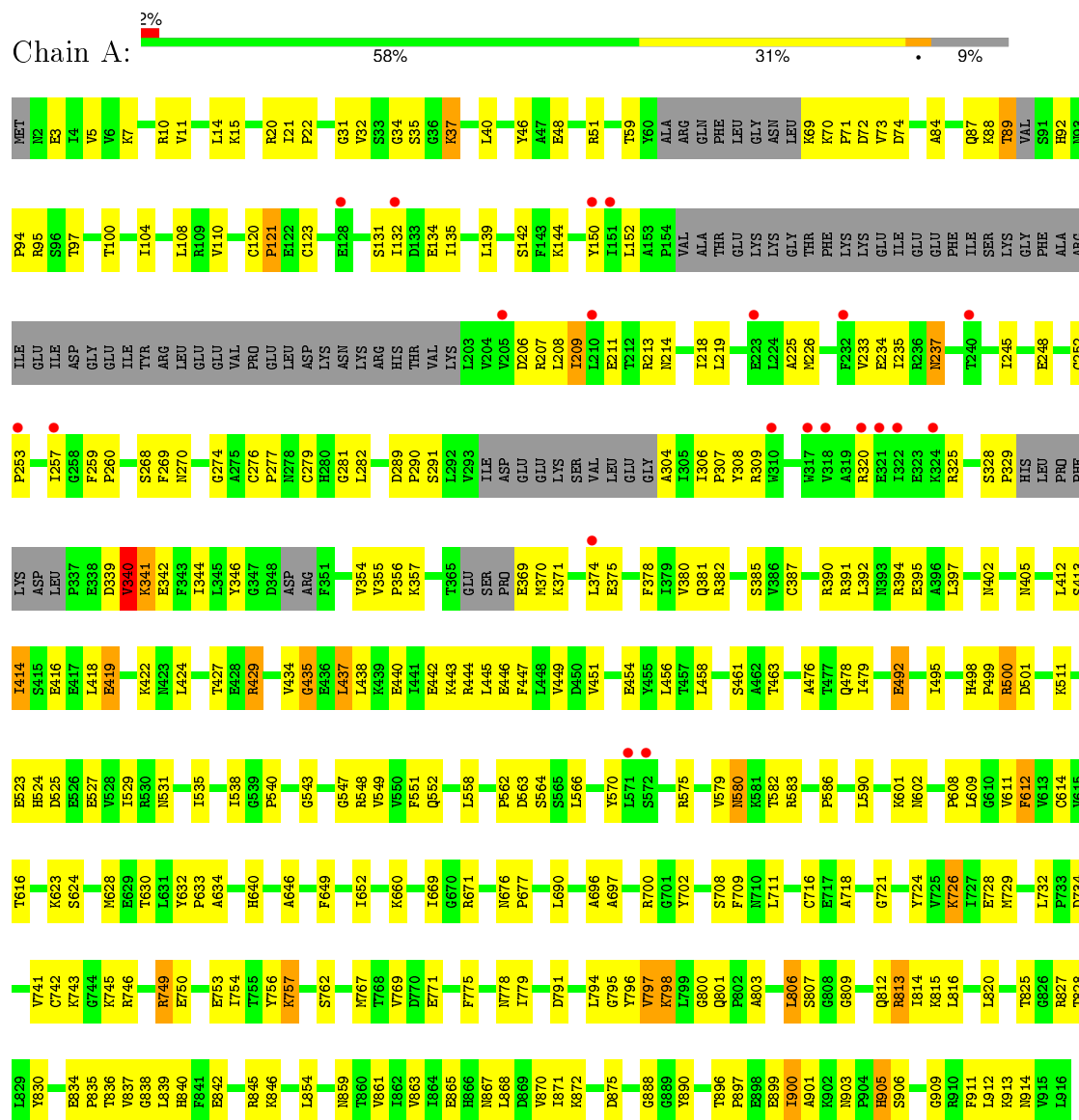
- Molecule 5 is water.

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

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.

• Molecule 1: UvrABC system protein A



• 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 48.35 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.5 (48.08-2.90) 96.0 (48.35-2.90)	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 0.200 , 0.267	Depositor DCC
R_{free} test set	1312 reflections (5.25%)	DCC
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 , 53.8	EDS
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
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 26298 reflections	Xtriage
F_o, F_c correlation	0.93	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.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.33	0/6499	0.52	0/8797
2	D	0.65	0/732	1.42	9/1128 (0.8%)
All	All	0.38	0/7231	0.69	9/9925 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	27	DA	O4'-C4'-C3'	-8.94	100.63	106.00
2	D	15	DC	O4'-C1'-N1	8.62	114.03	108.00
2	D	25	DT	O4'-C1'-N1	-6.28	103.61	108.00
2	D	26	DG	O4'-C1'-C2'	-6.13	101.00	105.90
2	D	32	DT	N3-C4-O4	5.65	123.29	119.90
2	D	13	DT	O4'-C4'-C3'	-5.22	102.41	104.50
2	D	10	DT	C1'-O4'-C4'	-5.17	104.93	110.10
2	D	14	DT	C5-C4-O4	-5.10	121.33	124.90
2	D	12	DG	O4'-C4'-C3'	-5.01	102.50	104.50

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	228	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	251	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 18.

All (251) 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:414:ILE:HD11	1:A:449:VAL:HG23	1.70	0.73
1:A:340:VAL:HG13	1:A:340:VAL:O	1.88	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:813:ARG:HD3	1:A:839:LEU:HD21	1.71	0.71
1:A:729:MET:HB2	1:A:732:LEU:HD11	1.72	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:PRO:HG3	1:A:608:PRO:HB3	1.79	0.65
1:A:525:ASP:O	1:A:529:ILE:HG13	1.97	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:209:ILE:HG22	1:A:211:GLU:HG3	1.81	0.62
2:D:12:DG:H1'	2:D:13:DT:C5'	2.30	0.61
1:A:498:HIS:ND1	1:A:499:PRO:HD2	2.15	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: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
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:HD12	1:A:779:ILE:N	2.17	0.60
1:A:812:GLN:HG2	5:A:938:HOH:O	2.01	0.58
1:A:562:PRO:C	1:A:564:SER:H	2.05	0.58
1:A:121:PRO:HD2	1:A:257:ILE:HD11	1.84	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
2:D:17:DG:H1'	2:D:18:DG:H5'	1.85	0.57
1:A:444:ARG:HA	1:A:447:PHE:CD2	2.39	0.57
1:A:104:ILE:HD13	1:A:445:LEU:HD12	1.87	0.56
1:A:237:ASN:HD22	1:A:237:ASN:C	2.07	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ASN:ND2	1:A:800:GLY:HA2	2.22	0.54
1:A:440:GLU:O	1:A:443:LYS:HG2	2.08	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:690:LEU:C	1:A:690:LEU:HD23	2.28	0.53
1:A:726:LYS:HB3	1:A:726:LYS:NZ	2.23	0.53
1:A:88:LYS:O	1:A:89:THR:C	2.47	0.53
2:D:31:DC:H3'	2:D:32:DT:H71	1.89	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
2:D:1:DA:H8	2:D:1:DA:O5'	1.91	0.53
1:A:15:LYS:HG2	1:A:548:ARG:HH11	1.73	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
2:D:2:DG:C8	2:D:3:DT:H72	2.44	0.52
1:A:660:LYS:CB	1:A:828:THR:HG22	2.38	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:632:TYR:HB3	1:A:633:PRO:HD3	1.90	0.52
1:A:543:GLY:N	1:A:796:TYR:CE1	2.78	0.52
2:D:10:DT:H2''	2:D:11:DG:C8	2.45	0.52
1:A:442:GLU:O	1:A:446:GLU:HG3	2.09	0.52
1:A:281:GLY:HA2	1:A:391:ARG:O	2.10	0.52
1:A:803:ALA:O	1:A:806:LEU:HB2	2.10	0.52
1:A:690:LEU:HD21	1:A:756:TYR:CD1	2.45	0.52
1:A:135:ILE:O	1:A:139:LEU:HG	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:579:VAL:O	1:A:580:ASN:C	2.48	0.51
1:A:281:GLY:O	1:A:391:ARG:HD3	2.10	0.51
1:A:269:PHE:HB3	1:A:392:LEU:HD23	1.92	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:339:ASP:O	1:A:340:VAL:HB	2.11	0.50
1:A:289:ASP:HB2	1:A:380:VAL:CG1	2.41	0.50
1:A:825:THR:OG1	1:A:828:THR:HG23	2.10	0.50
2:D:10:DT:H2''	2:D:11:DG:H8	1.76	0.50
1:A:601:LYS:HE2	1:A:888:GLY:O	2.11	0.50
1:A:97:THR:OG1	1:A:100:THR:HG23	2.10	0.50
1:A:676:ASN:HB2	1:A:677:PRO:HD2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:VAL:HB	1:A:795:GLY:HA2	1.93	0.50
2:D:12:DG:C8	2:D:12:DG:H5'	2.47	0.50
1:A:498:HIS:CG	1:A:499:PRO:HD2	2.47	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:381:GLN:HG3	1:A:381:GLN:O	2.12	0.49
1:A:95:ARG:HD3	1:A:270:ASN:OD1	2.13	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
2:D:18:DG:C2'	2:D:19:DA:C8	2.95	0.49
1:A:716:CYS:SG	1:A:742:CYS:HB3	2.53	0.49
1:A:414:ILE:HG13	1:A:454:GLU:HA	1.95	0.48
1:A:729:MET:HB2	1:A:732:LEU:CD1	2.43	0.48
1:A:608:PRO:HB2	1:A:611:VAL:CG2	2.44	0.48
1:A:909:GLY:O	1:A:913:LYS:HG3	2.12	0.48
1:A:32:VAL:HA	1:A:840:HIS:CB	2.43	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:562:PRO:C	1:A:564:SER:N	2.67	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:767:MET:HB2	1:A:771:GLU:HB3	1.95	0.47
1:A:59:THR:HG21	5:A:932:HOH:O	2.14	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: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:500:ARG:O	1:A:500:ARG:HG2	2.14	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:289:ASP:C	1:A:291:SER:H	2.18	0.46
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
2:D:3:DT:C2'	2:D:4:DG:C8	2.91	0.46
1:A:31:GLY:N	1:A:37:LYS:HE3	2.30	0.46
2:D:18:DG:C5'	2:D:18:DG:C8	2.98	0.46
1:A:575:ARG:HH11	1:A:845:ARG:NH2	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:HG2	1:A:213:ARG:O	2.14	0.46
1:A:422:LYS:C	1:A:424:LEU:H	2.19	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
2:D:18:DG:H2"	2:D:19:DA:H8	1.79	0.46
1:A:397:LEU:CA	1:A:405:ASN:HD22	2.29	0.46
1:A:896:THR:OG1	1:A:899:GLU:HG3	2.14	0.46
1:A:634:ALA:HB1	1:A:652:ILE:HD11	1.98	0.46
1:A:268:SER:O	1:A:274:GLY:HA3	2.16	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:307:PRO:HB3	1:A:378:PHE:CD2	2.51	0.45
1:A:5:VAL:HG22	1:A:20:ARG:HG2	1.98	0.45
1:A:535:ILE:O	1:A:552:GLN:HA	2.16	0.45
1:A:745:LYS:C	1:A:746:ARG:HG2	2.37	0.45
1:A:32:VAL:HA	1:A:840:HIS:HB2	1.98	0.45
1:A:340:VAL:CG1	1:A:340:VAL:O	2.58	0.45
1:A:226:MET:SD	1:A:248:GLU:HB3	2.56	0.45
1:A:562:PRO:O	1:A:564:SER:N	2.50	0.45
1:A:449:VAL:HG22	1:A:454:GLU:HB3	1.98	0.45
1:A:15:LYS:HB2	1:A:547:GLY:O	2.17	0.45
1:A:798:LYS:HB3	1:A:798:LYS:HE2	1.73	0.44
1:A:728:GLU:HG2	1:A:734:ASP:OD1	2.17	0.44
1:A:37:LYS:H	1:A:37:LYS:HG3	1.64	0.44
1:A:527:GLU:O	1:A:531:ASN:ND2	2.47	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:48:GLU:HA	1:A:48:GLU:OE1	2.17	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:51:ARG:HH11	1:A:70:LYS:HA	1.83	0.44
1:A:87:GLN:CD	1:A:87:GLN:H	2.17	0.44
1:A:743:LYS:HE3	1:A:745:LYS:HG3	1.98	0.44
1:A:94:PRO:HB2	1:A:282:LEU:HD22	2.00	0.44
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:628:MET:HE2	1:A:628:MET:HB3	1.92	0.43
1:A:21:ILE:HA	1:A:22:PRO:HD3	1.90	0.43
1:A:867:ASN:O	1:A:871:ILE:HG13	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:551:PHE:CZ	1:A:558:LEU:HB2	2.54	0.43
1:A:794:LEU:HD12	1:A:794:LEU:HA	1.83	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: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:583:ARG:HG3	1:A:875:ASP:HA	2.00	0.42
1:A:414:ILE:HG12	1:A:454:GLU:HA	2.02	0.42
1:A:276:CYS:SG	1:A:277:PRO:HD2	2.59	0.42
1:A:208:LEU:HD23	1:A:208:LEU:N	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:434:VAL:O	1:A:435:GLY:C	2.58	0.42
1:A:15:LYS:HG2	1:A:548:ARG:NH1	2.34	0.42
1:A:3:GLU:HB2	1:A:21:ILE:O	2.19	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:630:THR:O	1:A:633:PRO:HD2	2.20	0.42
1:A:523:GLU:HG3	1:A:524:HIS:N	2.35	0.42
1:A:120:CYS:SG	1:A:257:ILE:HD11	2.60	0.42
1:A:511:LYS:HE3	1:A:511:LYS:HB2	1.72	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:813:ARG:CD	1:A:839:LEU:HD21	2.44	0.41
1:A:97:THR:HB	1:A:458:LEU:O	2.20	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:806:LEU:HD12	1:A:806:LEU:HA	1.82	0.41
1:A:276:CYS:HA	1:A:277:PRO:HD3	1.91	0.41
2:D:24:DC:H2'	2:D:25:DT:H72	2.02	0.41
1:A:836:THR:HG21	1:A:870:VAL:HG21	2.02	0.41
1:A:601:LYS:O	1:A:602:ASN:C	2.58	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:H	1:A:779:ILE:HD12	1.85	0.41
1:A:131:SER:OG	1:A:134:GLU:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ARG:HB2	1:A:911:PHE:CE2	2.56	0.41
1:A:259:PHE:HA	1:A:260:PRO:HD3	1.89	0.41
1:A:150:TYR:CE2	1:A:207:ARG:HB2	2.56	0.40
1:A:749:ARG:HG2	1:A:750:GLU:N	2.35	0.40
1:A:11:VAL:O	1:A:14:LEU:HB2	2.20	0.40
1:A:900:ILE:HG22	1:A:912:LEU:HD23	2.03	0.40
1:A:612:PHE:C	1:A:612:PHE:CD2	2.94	0.40
1:A:339:ASP:O	1:A:340:VAL:CB	2.69	0.40
1:A:586:PRO:HA	1:A:609:LEU:O	2.21	0.40
1:A:418:LEU:O	1:A:422:LYS:HD3	2.20	0.40
1:A:304:ALA:N	1:A:309:ARG:HE	2.19	0.40
1:A:46:TYR:CD1	1:A:84:ALA:HB2	2.56	0.40
1:A:709:PHE:CD2	1:A:709:PHE:C	2.94	0.40
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.83	0.40
1:A:816:LEU:HG	1:A:820:LEU:HD12	2.04	0.40
1:A:306:ILE:N	1:A:307:PRO:CD	2.85	0.40
1:A:612:PHE:C	1:A:612:PHE:HD2	2.24	0.40
1:A:252:CYS:HA	1:A:253:PRO:HD3	1.86	0.40

There are no symmetry-related clashes.

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	820/916 (90%)	739 (90%)	72 (9%)	9 (1%)	<div><div>17</div><div>51</div></div>

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	VAL
1	A	435	GLY
1	A	775	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	637 (94%)	44 (6%)	21	52

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	89	THR
1	A	92	HIS
1	A	142	SER
1	A	144	LYS
1	A	209	ILE
1	A	237	ASN
1	A	279	CYS
1	A	320	ARG
1	A	325	ARG
1	A	340	VAL
1	A	341	LYS
1	A	382	ARG
1	A	385	SER
1	A	394	ARG
1	A	414	ILE
1	A	419	GLU
1	A	427	THR
1	A	429	ARG
1	A	437	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	451	VAL
1	A	478	GLN
1	A	492	GLU
1	A	500	ARG
1	A	580	ASN
1	A	582	THR
1	A	590	LEU
1	A	612	PHE
1	A	624	SER
1	A	640	HIS
1	A	726	LYS
1	A	749	ARG
1	A	762	SER
1	A	778	ASN
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	900	ILE
1	A	905	HIS
1	A	906	SER
1	A	914	ASN

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	2	ASN
1	A	214	ASN
1	A	216	HIS
1	A	237	ASN
1	A	249	ASN
1	A	657	ASN
1	A	812	GLN

5.3.3 RNA ⓘ

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 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	0.88	0	11,13,13	1.43	1 (9%)
3	PPV	A	1002	-	6,8,8	0.88	0	11,13,13	1.16	1 (9%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	PPV	P2-OPP-P1	-4.02	119.19	132.67
3	A	1002	PPV	P2-OPP-P1	-2.63	123.86	132.67

There are no chirality outliers.

There are no torsion outliers.

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

6.1 Protein, DNA and RNA chains

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%)	-0.06	21 (2%) 61 55	30, 61, 96, 114	0
2	D	32/32 (100%)	0.64	5 (15%) 3 1	46, 76, 89, 108	0
All	All	868/948 (91%)	-0.03	26 (2%) 54 47	30, 62, 96, 114	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	PRO	3.8
2	D	1	DA	3.5
1	A	310	TRP	3.5
1	A	321	GLU	3.3
1	A	232	PHE	3.2
1	A	572	SER	3.1
1	A	257	ILE	3.0
2	D	15	DC	2.9
1	A	128	GLU	2.8
1	A	324	LYS	2.8
2	D	16	DC	2.7
2	D	20	DA	2.5
1	A	205	VAL	2.5
1	A	322	ILE	2.5
1	A	317	TRP	2.4
1	A	210	LEU	2.4
1	A	223	GLU	2.3
1	A	320	ARG	2.3
1	A	374	LEU	2.3
1	A	318	VAL	2.2
1	A	571	LEU	2.2
1	A	132	ILE	2.2
1	A	240	THR	2.1
1	A	150	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	31	DC	2.1
1	A	151	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	PPV	A	1001	9/9	0.97	0.20	1.37	46,51,103,119	0
4	ZN	A	918	1/1	0.97	0.15	0.43	70,70,70,70	0
4	ZN	A	917	1/1	0.99	0.16	0.30	68,68,68,68	0
4	ZN	A	919	1/1	0.99	0.09	-1.36	80,80,80,80	1
3	PPV	A	1002	9/9	0.96	0.15	-1.41	52,67,81,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.