



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:48 PM GMT

PDB ID : 4AJW
Title : Discovery and Optimization of New Benzimidazole- and Benzoxazole-Pyrimidone Selective PI3KBeta Inhibitors for the Treatment of Phosphatase and TENSin homologue (PTEN)-Deficient Cancers"
Authors : Certal, V.; Halley, F.; Virone-Oddos, A.; Delorme, C.; Karlsson, A.; Rak, A.; Thompson, F.; Filoche-Romme, B.; El-Ahmad, Y.; Carry, J.C.; Abecassis, P.Y.; Lejeune, P.; Bonnevaux, H.; Nicolas, J.P.; Bertrand, T.; Marquette, J.P.; Michot, N.; Benard, T.; Below, P.; Vade, I.; Chatreaux, F.; Lebourg, G.; Pilorge, F.; Angouillant-Boniface, O.; Louboutin, A.; Lengauer, C.; Schio, L.
Deposited on : 2012-02-20
Resolution : 2.80 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

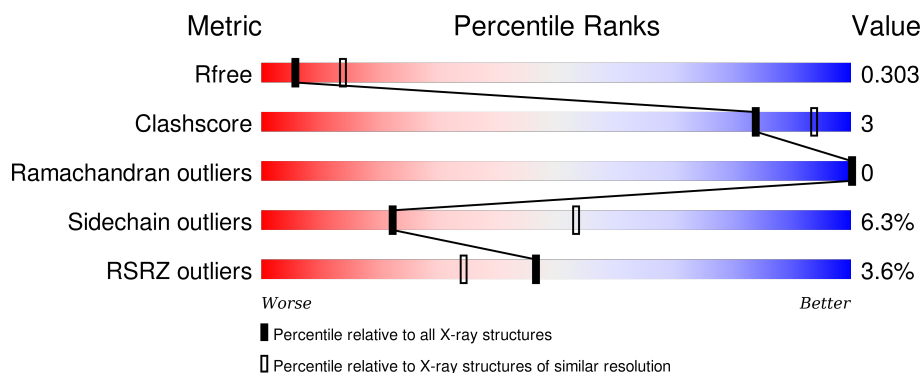
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

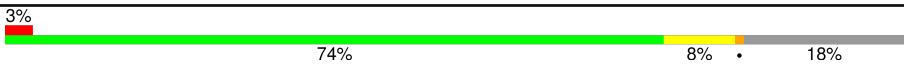

The reported resolution of this entry is 2.80 Å.

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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	934	
1	B	934	

2 Entry composition [i](#)

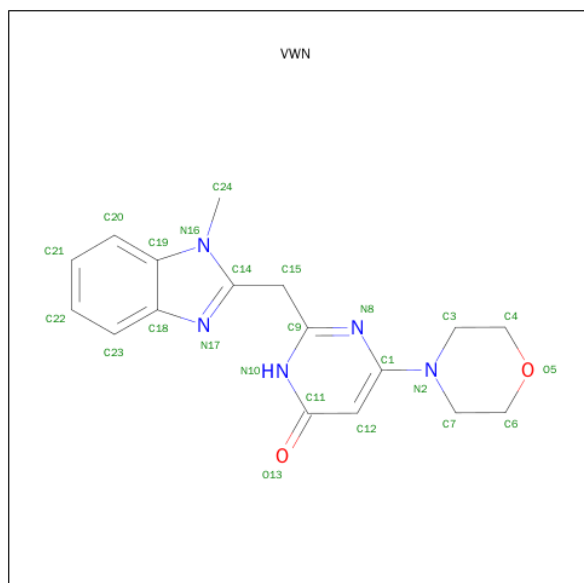
There are 3 unique types of molecules in this entry. The entry contains 12596 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			6151	3942	1042	1116	51			
1	B	792	Total	C	N	O	S	0	0	0
			6363	4076	1076	1158	53			

- Molecule 2 is 2-[(1-METHYL-1H-BENZIMIDAZOL-2-YL)METHYL]-6-MORPHOLIN-4-YPYRIMIDIN-4(3H)-ONE (three-letter code: VWN) (formula: C₁₇H₁₉N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	17	5	2		
2	B	1	Total	C	N	O	0	0
			24	17	5	2		

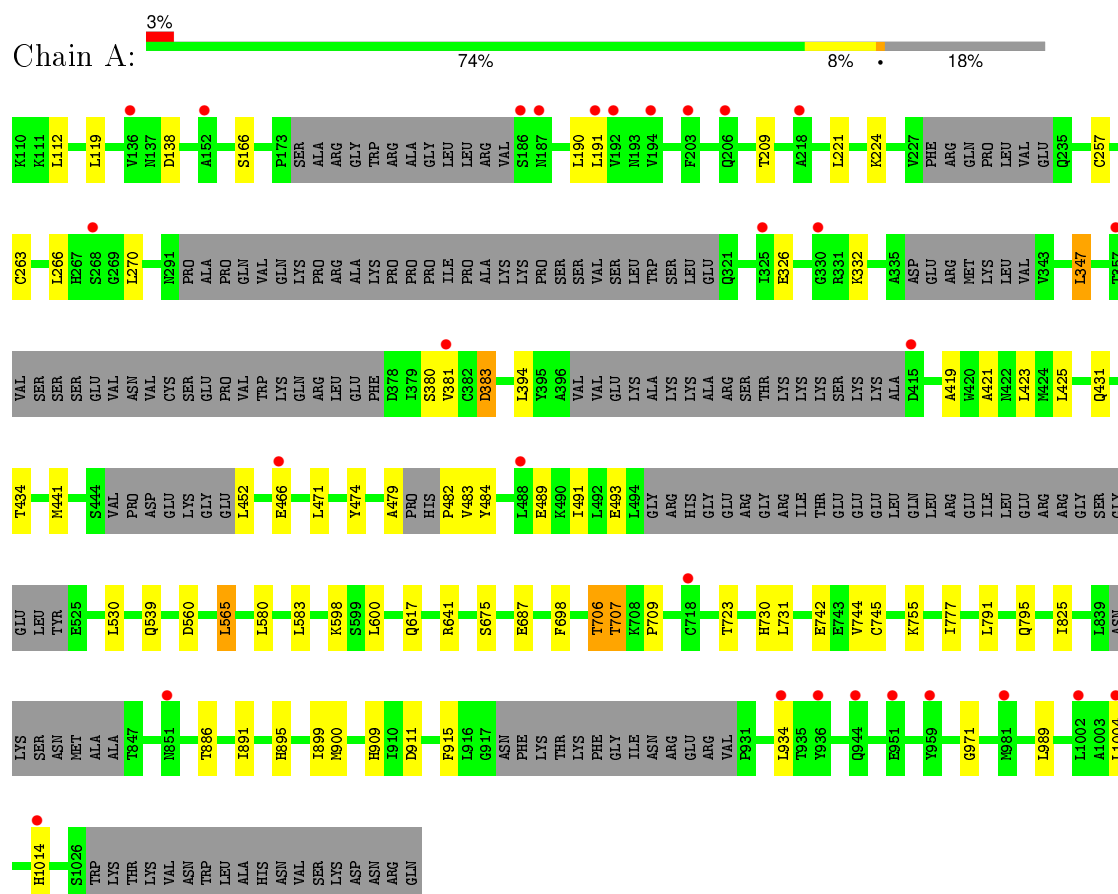
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0
3	B	15	Total 15	O 15	0	0

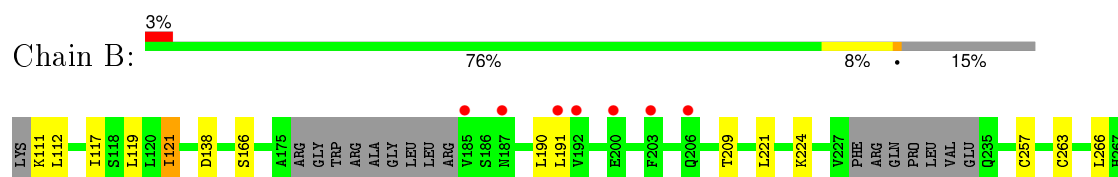
3 Residue-property plots

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: PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM



• Molecule 1: PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.40Å 220.47Å 78.26Å 90.00° 113.87° 90.00°	Depositor
Resolution (Å)	71.57 – 2.80 110.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (71.57-2.80) 98.4 (110.23-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.82Å)	Xtriage
Refinement program	BUSTER-TNT 2.9.7	Depositor
R, R_{free}	0.252 , 0.277 0.281 , 0.303	Depositor DCC
R_{free} test set	2414 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.5	EDS
Estimated twinning fraction	0.457 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 47495 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12596	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1/6282 (0.0%)	0.55	0/8470
1	B	0.45	1/6499 (0.0%)	0.55	0/8767
All	All	0.44	2/12781 (0.0%)	0.55	0/17237

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	745	CYS	CB-SG	-6.57	1.71	1.82
1	A	745	CYS	CB-SG	-5.03	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6151	0	6129	32	0
1	B	6363	0	6340	42	0
2	A	24	0	19	1	0
2	B	24	0	19	1	0
3	A	19	0	0	0	0
3	B	15	0	0	0	0
All	All	12596	0	12507	74	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 3.

All (74) 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:B:753:ASP:CG	1:B:757:LYS:NZ	2.08	1.08
1:B:753:ASP:HA	1:B:757:LYS:HZ2	1.32	0.91
1:B:753:ASP:HA	1:B:757:LYS:NZ	1.85	0.90
1:A:707:THR:OG1	1:A:709:PRO:HD2	1.74	0.86
1:B:753:ASP:CG	1:B:757:LYS:HZ1	1.79	0.86
1:A:989:LEU:O	1:A:989:LEU:HG	1.75	0.84
1:B:431:GLN:HG3	1:B:484:TYR:CE1	2.16	0.81
1:A:483:VAL:CG2	1:A:483:VAL:O	2.30	0.80
1:A:483:VAL:HG22	1:A:483:VAL:O	1.82	0.78
1:B:989:LEU:HG	1:B:989:LEU:O	1.87	0.75
1:A:431:GLN:HG3	1:A:484:TYR:CE1	2.21	0.75
1:A:730:HIS:HD2	1:A:742:GLU:OE1	1.70	0.74
1:B:483:VAL:O	1:B:483:VAL:CG2	2.36	0.73
1:B:753:ASP:CA	1:B:757:LYS:HZ2	2.03	0.72
1:B:753:ASP:OD2	1:B:757:LYS:NZ	2.18	0.71
1:B:753:ASP:CA	1:B:757:LYS:NZ	2.54	0.71
1:B:117:ILE:O	1:B:121:ILE:HG23	1.89	0.71
1:B:431:GLN:HG3	1:B:484:TYR:CD1	2.34	0.62
1:A:431:GLN:HG3	1:A:484:TYR:CD1	2.34	0.62
1:A:479:ALA:HB3	1:A:482:PRO:HD2	1.81	0.61
1:A:706:THR:OG1	1:A:707:THR:N	2.29	0.60
1:B:483:VAL:O	1:B:483:VAL:HG22	2.02	0.60
1:B:989:LEU:CG	1:B:989:LEU:O	2.45	0.59
1:A:479:ALA:CB	1:A:482:PRO:HD2	2.32	0.59
1:B:421:ALA:HB2	1:B:441:MET:HG2	1.84	0.59
1:B:753:ASP:CG	1:B:757:LYS:HZ3	2.07	0.56
1:B:753:ASP:CG	1:B:757:LYS:HZ2	2.05	0.55
1:B:753:ASP:CB	1:B:757:LYS:NZ	2.70	0.54
1:B:753:ASP:CB	1:B:757:LYS:HZ2	2.21	0.54
1:A:479:ALA:HB3	1:A:482:PRO:CD	2.39	0.53
1:A:421:ALA:HB2	1:A:441:MET:HG2	1.91	0.53
1:A:989:LEU:O	1:A:989:LEU:CG	2.45	0.53
1:A:431:GLN:HA	1:A:484:TYR:HA	1.92	0.52
1:B:989:LEU:HD12	1:B:989:LEU:C	2.30	0.52
1:B:347:LEU:HD21	1:B:425:LEU:HD11	1.91	0.52
1:B:483:VAL:HG23	1:B:483:VAL:O	2.09	0.51
1:A:380:SER:HB3	1:A:383:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LEU:HD21	1:A:425:LEU:HD11	1.91	0.51
1:A:899:ILE:HG12	1:A:909:HIS:CE1	2.47	0.50
1:A:491:ILE:HG21	1:A:565:LEU:HD22	1.94	0.50
1:B:491:ILE:HG21	1:B:565:LEU:HD22	1.94	0.49
1:B:911:ASP:OD1	1:B:911:ASP:O	2.30	0.49
1:B:753:ASP:HA	1:B:757:LYS:HZ3	1.76	0.48
1:A:479:ALA:C	1:A:482:PRO:HD3	2.34	0.48
1:B:886:THR:HA	1:B:891:ILE:HD12	1.96	0.47
1:A:209:THR:HG22	1:A:257:CYS:HB3	1.96	0.47
1:A:886:THR:HA	1:A:891:ILE:HD12	1.96	0.47
1:A:263:CYS:HA	1:A:266:LEU:HD12	1.98	0.47
1:B:326:GLU:HB3	1:B:474:TYR:HB3	1.98	0.46
1:B:692:LEU:HG	1:B:728:LEU:HD21	1.97	0.45
1:A:326:GLU:HB3	1:A:474:TYR:HB3	1.98	0.45
1:B:263:CYS:HA	1:B:266:LEU:HD12	1.98	0.45
1:B:209:THR:HG22	1:B:257:CYS:HB3	1.99	0.45
1:A:730:HIS:CD2	1:A:742:GLU:OE1	2.61	0.44
1:A:707:THR:OG1	1:A:709:PRO:CD	2.56	0.44
1:B:434:THR:HA	1:B:435:GLY:HA2	1.77	0.44
1:A:777:ILE:HB	1:A:825:ILE:HB	1.99	0.43
1:A:580:LEU:HA	1:A:583:LEU:HD12	2.01	0.43
1:A:419:ALA:HB1	1:A:441:MET:HB3	2.01	0.43
1:B:752:MET:O	1:B:757:LYS:HA	2.18	0.42
1:A:900:MET:SD	2:A:2027:VWN:H72C	2.59	0.42
1:B:691:LYS:HE3	1:B:723:THR:HB	2.01	0.42
1:B:753:ASP:CA	1:B:757:LYS:HZ3	2.28	0.42
1:B:580:LEU:HA	1:B:583:LEU:HD12	2.01	0.42
1:B:971:GLY:HA3	1:B:1004:LEU:HD11	2.02	0.42
1:B:900:MET:SD	2:B:2027:VWN:H72C	2.60	0.42
1:B:759:LEU:HB2	1:B:778:PHE:HB3	2.02	0.42
1:B:777:ILE:HB	1:B:825:ILE:HB	2.02	0.42
1:B:583:LEU:HD11	1:B:600:LEU:HD11	2.03	0.41
1:B:328:ILE:HD11	1:B:474:TYR:HB2	2.02	0.41
1:A:730:HIS:H	1:A:742:GLU:HA	1.86	0.41
1:B:750:THR:OG1	1:B:751:PHE:N	2.54	0.41
1:A:971:GLY:HA3	1:A:1004:LEU:HD11	2.02	0.41
1:A:583:LEU:HD11	1:A:600:LEU:HD11	2.02	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	741/934 (79%)	718 (97%)	23 (3%)	0	100	100
1	B	770/934 (82%)	746 (97%)	24 (3%)	0	100	100
All	All	1511/1868 (81%)	1464 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	674/823 (82%)	630 (94%)	44 (6%)	21	52
1	B	700/823 (85%)	657 (94%)	43 (6%)	23	55
All	All	1374/1646 (84%)	1287 (94%)	87 (6%)	22	53

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	119	LEU
1	A	138	ASP
1	A	166	SER
1	A	190	LEU
1	A	191	LEU
1	A	221	LEU
1	A	224	LYS

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Mol	Chain	Res	Type
1	A	270	LEU
1	A	332	LYS
1	A	347	LEU
1	A	381	VAL
1	A	383	ASP
1	A	394	LEU
1	A	423	LEU
1	A	434	THR
1	A	452	LEU
1	A	466	GLU
1	A	471	LEU
1	A	489	GLU
1	A	493	GLU
1	A	530	LEU
1	A	539	GLN
1	A	560	ASP
1	A	565	LEU
1	A	598	LYS
1	A	617	GLN
1	A	641	ARG
1	A	675	SER
1	A	687	GLU
1	A	698	PHE
1	A	706	THR
1	A	707	THR
1	A	723	THR
1	A	731	LEU
1	A	744	VAL
1	A	755	LYS
1	A	791	LEU
1	A	795	GLN
1	A	895	HIS
1	A	911	ASP
1	A	915	PHE
1	A	934	LEU
1	A	1014	HIS
1	B	111	LYS
1	B	112	LEU
1	B	119	LEU
1	B	121	ILE
1	B	138	ASP
1	B	166	SER

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Mol	Chain	Res	Type
1	B	190	LEU
1	B	191	LEU
1	B	221	LEU
1	B	224	LYS
1	B	270	LEU
1	B	332	LYS
1	B	341	LEU
1	B	347	LEU
1	B	374	ARG
1	B	380	SER
1	B	383	ASP
1	B	394	LEU
1	B	423	LEU
1	B	434	THR
1	B	466	GLU
1	B	471	LEU
1	B	483	VAL
1	B	489	GLU
1	B	493	GLU
1	B	530	LEU
1	B	539	GLN
1	B	560	ASP
1	B	565	LEU
1	B	598	LYS
1	B	617	GLN
1	B	675	SER
1	B	687	GLU
1	B	723	THR
1	B	731	LEU
1	B	744	VAL
1	B	755	LYS
1	B	791	LEU
1	B	795	GLN
1	B	895	HIS
1	B	915	PHE
1	B	934	LEU
1	B	1014	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	HIS

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Mol	Chain	Res	Type
1	A	610	GLN
1	A	730	HIS
1	A	732	GLN
1	A	786	GLN
1	A	906	GLN
1	B	258	HIS
1	B	610	GLN
1	B	780	ASN
1	B	786	GLN
1	B	906	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](#)

2 ligands are 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	VWN	A	2027	-	22,27,27	1.42	3 (13%)	27,38,38	1.93	4 (14%)
2	VWN	B	2027	-	22,27,27	1.42	3 (13%)	27,38,38	1.93	4 (14%)

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	VWN	A	2027	-	-	0/8/16/16	0/4/4/4
2	VWN	B	2027	-	-	0/8/16/16	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2027	VWN	C1-N2	2.22	1.42	1.37
2	B	2027	VWN	C1-N2	2.23	1.42	1.37
2	A	2027	VWN	C11-N10	3.02	1.38	1.33
2	B	2027	VWN	C11-N10	3.06	1.38	1.33
2	B	2027	VWN	C9-N10	4.28	1.40	1.33
2	A	2027	VWN	C9-N10	4.35	1.40	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2027	VWN	C12-C11-N10	-7.49	114.97	124.05
2	B	2027	VWN	C12-C11-N10	-7.46	115.00	124.05
2	A	2027	VWN	C24-N16-C14	2.83	130.56	125.22
2	B	2027	VWN	C24-N16-C14	2.85	130.60	125.22
2	B	2027	VWN	C9-N8-C1	3.02	118.20	115.68
2	A	2027	VWN	C9-N8-C1	3.03	118.21	115.68
2	B	2027	VWN	C11-C12-C1	4.06	121.40	116.33
2	A	2027	VWN	C11-C12-C1	4.08	121.44	116.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2027	VWN	1	0
2	B	2027	VWN	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	765/934 (81%)	0.38	29 (3%)	44 32	46, 71, 103, 124	5 (0%)
1	B	792/934 (84%)	0.42	27 (3%)	49 36	44, 73, 102, 129	5 (0%)
All	All	1557/1868 (83%)	0.40	56 (3%)	46 34	44, 72, 103, 129	10 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	ASN	4.3
1	B	934	LEU	3.8
1	A	936	TYR	3.8
1	B	185	VAL	3.6
1	A	934	LEU	3.4
1	B	470	ALA	3.4
1	B	1014	HIS	3.3
1	B	341	LEU	3.3
1	A	191	LEU	3.3
1	B	268	SER	3.2
1	A	1004	LEU	3.1
1	A	206	GLN	3.1
1	B	206	GLN	3.1
1	A	203	PHE	3.0
1	B	705	LYS	3.0
1	B	718	CYS	2.9
1	A	357	THR	2.8
1	A	192	VAL	2.8
1	B	330	GLY	2.7
1	B	203	PHE	2.6
1	B	334	ASN	2.6
1	B	466	GLU	2.6
1	B	714	MET	2.6
1	B	191	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	851	ASN	2.5
1	A	944	GLN	2.5
1	A	187	ASN	2.5
1	B	962	ARG	2.5
1	A	218	ALA	2.4
1	A	381	VAL	2.4
1	A	268	SER	2.4
1	A	1014	HIS	2.4
1	A	330	GLY	2.3
1	B	1004	LEU	2.3
1	A	325	ILE	2.3
1	A	718	CYS	2.3
1	B	708	LYS	2.3
1	B	200	GLU	2.2
1	A	959	TYR	2.2
1	B	271	THR	2.2
1	A	981	MET	2.2
1	B	745	CYS	2.2
1	A	136	VAL	2.2
1	B	851	ASN	2.2
1	A	186	SER	2.1
1	A	1002	LEU	2.1
1	B	192	VAL	2.1
1	A	152	ALA	2.1
1	A	194	VAL	2.1
1	B	981	MET	2.1
1	A	415	ASP	2.1
1	A	951	GLU	2.1
1	B	836	ASN	2.1
1	A	488	LEU	2.1
1	B	332	LYS	2.0
1	A	466	GLU	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
2	VWN	B	2027	24/24	0.93	0.29	1.25	72,73,73,74	0
2	VWN	A	2027	24/24	0.91	0.29	0.88	80,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.